

Light Nuclei Systematics in the Unrestricted Hartree–Fock Approximation

H. C. LEE AND R. Y. CUSSON*

*Chalk River Nuclear Laboratories, Atomic Energy of Canada Limited,
Chalk River, Ontario, Canada*

Received June 18, 1971

Extensive unrestricted Hartree–Fock (HF) calculations have been performed for 57 light nuclei in the region $4 \leq A \leq 41$, $N - Z = 0, \pm 1$. An expansion basis consisting of the first 5 major shells plus the $0h_{11/2}$ subshell of the j - j coupled spherical harmonic oscillator model is used, so that 82 proton and 82 neutron states are considered. The semirealistic N - N interaction No. 2 of Saunier and Pearson is used and seen to be a reasonable energy- and density-independent approximation to the required reaction matrix. All quantum numbers of the Hamiltonian are violated in the single-particle (sp) orbits, except parity and isospin projection τ_z . Time-reversal violation in the sp orbits is shown to be an important effect in odd and odd–odd nuclei and accounts for most of the odd–even pairing energy differences, although no pairing correlations are considered explicitly. No projection from the intrinsic states is performed, but its probable effects are discussed. The Coulomb two-body interaction is included and its matrix elements are computed exactly using Talmi integrals. The kinetic energy of the center-of-mass (c.m.) is removed from H before the HF iterations and rms radii are computed with respect to the c.m. so that spurious c.m. effects are minimized. Nilsson model wavefunctions are used as initial trial wavefunctions and shown to be good approximations for the HF wavefunctions. Reasonable-to-good agreement with experiment is obtained for the systematics of binding energies, separation energies, rms radii, electric quadrupole moments, and Coulomb energies. Alpha clustering is observed in the density distribution. New quantitative predictions are made for proton–neutron rms radii differences and isospin mixing coefficients, and compared with other calculations. It is concluded that a systematic quantitative account of the ground-state properties of the light nuclei can be given from a knowledge of the N - N interaction and nuclear matter properties alone.

1. INTRODUCTION

The properties of the light nuclei offer one of the most interesting challenges to the many-body theory of quantum systems since, in the region $4 \leq A \leq 40$ of

* Permanent address: Department of Physics, Duke University, Durham, NC 27706.

the periodic table, the effects of the transition from a complete microscopic description, in terms of an A -nucleon antisymmetrized wavefunction, to one where specific measurements confirm particular global models, are expected to be most noticeable. However, partly because of the intermediate structure involved and partly because of the apparent complexity of the nuclear interactions, most closed form approximations to these properties yield only qualitative agreement with experiment. In view of the theoretical importance of the subject and of the large amount of experimental data available, we shall present, in this paper, some of the results of large-scale numerical calculations which were aimed primarily at obtaining systematic quantitative predictions for the observable ground-state properties of these nuclei, such as binding energies, density distributions, Coulomb energies and separation energies, etc. It is hoped that this work will be of some use not only to experimentalists but also to theoretical physicists concerned with improving the formal methods of approximation in the light nuclides region.

We devote the rest of this Introduction to recalling the modern context of the Hartree-Fock approximation and some of the recent work in this area. Section 2 outlines the method and emphasizes selected points of interest in the calculation; Section 3 presents the main Table II and other results, while Section 4 discusses the results and their implication for future calculations.

If we let $H = T + v$ be the nuclear Hamiltonian consisting of the kinetic energy operator T and the two-body interaction potential v , the solution of the Schroedinger equation for the ground state wavefunction $|\Psi\rangle$,

$$H|\Psi\rangle = E|\Psi\rangle,$$

is in principle required for every nucleus in order to predict their systematics. We give a brief description of the structure of $|\Psi\rangle$, in order to appreciate its complexity and the methods of approximations which are in common use. The A -nucleon antisymmetrised $|\Psi\rangle$ belong to the A -fold product space of some single-particle basis space and may be expanded in antisymmetrised single Slater determinants [1] (SD), constructed on that single-particle basis of states $|\psi_\alpha\rangle$, $\alpha = 1, \dots, B$. Apart from the leading SD (the one with the largest amplitude) many others are needed, with smaller amplitudes, in order to obtain an accurate description. It has become increasingly clear, over the years that $|\Psi\rangle$ involves the following components: (i) the leading SD must be constructed from a large basis, $B \gg A$; (ii) highly excited two-particle two-hole ($2p-2h$) configurations must be included to account for the repulsive, singular, short-range part of the nuclear force; (iii) many coherent ($Np-Nh$) low-energy configurations will be required to describe the long-range and collective correlations. Starting from some convenient basis, in this case the j - j coupled harmonic oscillator basis, a unitary transformation may be performed on it, so that in the new one, which we label as $|\psi_i\rangle$,

$i = 1, \dots, B$, the expectation value ρ_{ij} on the exact $|\Psi\rangle$, of the single-particle density matrix operator [1], will be diagonal, namely,

$$\rho_{ij} = \delta_{ij}\rho_i,$$

where the ρ_i 's are the so called occupation probabilities. The effects of the various terms discussed above on the occupation probabilities is illustrated in Fig. 1. The

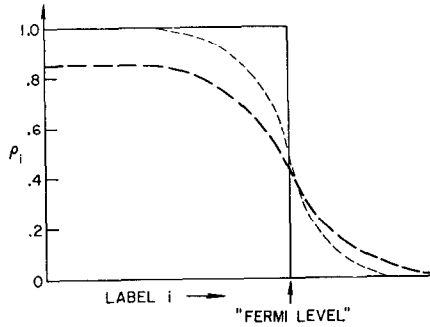


FIG. 1. The schematic density distributions for various wavefunctions $|\Psi\rangle$. The solid line represents the leading SD alone. The short-dashed line illustrates the effect of including type (iii) corrections while the long-dashed line shows a possible distribution resulting from all three components.

method of Hartree [2] and Fock [3] (HF) was originally proposed to obtain type (i) approximate states for electrons in atoms; this is thought to be a good approximation because the residual Coulomb interaction does not induce type (ii) corrections. For nuclei the effects of type (ii) corrections must be renormalised out of the interaction potential v , so that it is replaced by Breuckner's [4] K matrix, if we hope to represent $|\Psi\rangle$ using only type (i) and (iii) ingredients. This formally exact Breuckner-Hartree-Fock procedure has been applied successfully to closed-shell nuclei [5] and has the additional advantage of yielding better value for the occupation probabilities [6]. However, the double self-consistency implied by the method makes its application to other nuclei [7] very time-consuming. Now the renormalisation against type (ii) corrections is a short-range, high-energy effect and thus should not induce significant renormalization of operators which sample low-energy properties of $|\Psi\rangle$, such as the rms radius, etc. Most calculations have therefore assumed that one can write down at the outset an effective two-body operator, which we shall call v from now on, which would occupy the position of K , and yield good low-energy properties for the eigenstates of the resulting effective Hamiltonian $T + v$. This paper makes the same assumption and should therefore not be expected to make predictions about short-range effects.

The use of purely phenomenological simple expressions for v in restricted regions of the periodic table is described by Ripka [8] and has met with some success. It is only recently that more sophisticated forms for v have been found which appear to apply over the whole periodic table. To understand the applications of these forms we return briefly to our classification of the components of $|\Psi\rangle$. The HF leading SD is obtained as the variational solution to an energy minimisation problem. It therefore need not be an eigenfunction of all the operators which commute with H . The restoration of these symmetries may then be accomplished by using the Hill-Wheeler generator coordinate method [8] or "projection" method, and will introduce type (iii) corrections. This is not done here. Thus our results are restricted to properties which are not too sensitive to projection; the probable effects of this step will be discussed here, however. Several unrestricted HF calculations without projection have been performed [9, 10] using the Tabakin potential to represent the v discussed above. However, the results for the total binding energy are poor. On the other hand, excellent results for the binding energy of most spherical nuclei have been obtained recently [11, 12] by using density dependent phenomenological interactions. Still another approach, the one used here, consists in selecting a parametric form for v and adjusting these parameters to fit predetermined general criteria. The potentials of Nestor *et al.* [13] and those of Saunier and Pearson [14] are of this type. In particular, potential No. 2 of the latter authors is used here and represents a compromise in the simultaneous description of two-body properties and nuclear matter properties. Kuo [15] has discussed recently the problems of deriving energy-independent effective interactions from first principles; such a discussion is clearly beyond the scope of this paper.

The spherical harmonic oscillator basis used in this work is shown in Table I and includes the first five major shells ($N = 0-4$) plus the $0h_{11/2}$ orbit of the $N = 5$ shell so that 82 protons and 82 neutron orbitals are involved. This suffices to account for most of the quadrupole deformation components of the light nuclei ($A \leq 40$), without introducing one-body effective charges [8]. The 82 orbitals consists of 44 positive parity and 38 negative parity ones. Basis orbitals of different parity are not mixed in this calculation although there have been indications that such a mixing can take place [16, 17]. This point will be discussed further in Section III. The HF orbitals of the protons and the neutrons are not assumed to be the same so that isospin mixing is present and can be studied (Subsection 3.1). Each proton or neutron HF orbital of a given parity is allowed to mix all other-single-particle quantum numbers. An additional feature of the present calculation, which allows the treatment of odd-odd and odd nuclei, is that it is *not* assumed that *any* of the occupied orbits come in time-reversed pairs. In fact, all the wavefunctions are allowed to be complex although this feature is not crucial for the results reported here. In view of the very large number of variational parameters involved

TABLE I
The Single Particle Expansion Basis Used in This Work

I	n	l	j	$N = 2n + l$	$Z_{\text{cumulative}}$
16	1	2	3/2	4	82
15	0	5	11/2	5	
14	2	0	1/2	4	
13	0	4	7/2	4	
12	1	2	5/2	4	
11	0	4	9/2	4	50
10	1	1	1/2	3	40
9	0	3	5/2	3	
8	1	1	3/2	3	
7	0	3	7/2	3	28
6	0	2	3/2	2	20
5	1	0	1/2	2	
4	0	2	5/2	2	
3	0	1	1/2	1	8
2	0	1	3/2	1	
1	0	0	1/2	0	2

in this kind of calculation it is essential that very careful attention be paid to the problem of selecting the initial trial wavefunction for the iteration algorithm. For this purpose a preliminary study of the equilibrium deformation of the light nuclei in the ellipsoidal harmonic oscillator model of Mottelson [18] was made. A detailed program [19] (ELMOS) to solve the ellipsoidal harmonic oscillator model of Nilsson [20] was next undertaken. This resulted in a catalog [21] of the ground-state energy surface *vs.* β and γ of all the known isotopes of the light nuclei. It became clear at this point that several of those isotopes, because of the shallow energy surface, should also have some vibrational motion. Such motions are not studied here and in most cases we present the results obtained by selecting the initial wavefunction to be the one with the lowest energy in the Nilsson model. We have found generally good agreement between the deformation parameters in the Nilsson model and those of the HF results. The problems associated with spurious [22] c.m. states and motions were minimised by *removing* altogether the kinetic energy

TABLE II. Table For Representative HF Results^a

	⁴ He	⁵ He	⁵ He	⁵ Li	⁶ Li	⁷ Li	⁷ Be
$\hbar\omega$	20.0	20.0	17.5	17.5	17.5	17.5	17.5
β_o	0	0.20	0.20	0.20	0.42	0.56	0.56
γ_o	0	0	0	0	0	0	0
-W	28.198	22.802	23.053	21.956	22.345	30.001	28.375
W_c	0.857	0.831	0.825	1.914	1.891	1.811	3.443
$W_{c,D}$	1.711	1.662	1.649	3.105	3.079	2.998	5.051
ϵ_1^p	-22.52	-26.46	-25.99	-25.43	-30.88	-33.96	-28.30
ϵ_f^p	-22.52	-26.23	-25.82	1.38	-6.06	-13.53	-7.58
ϵ_{f+1}^p	5.38	1.20	0.77	3.44	-0.93	-7.45	1.67
ϵ_1^n	-23.32	-27.22	-26.84	-26.64	-32.21	-30.17	-35.12
ϵ_f^n	-23.32	0.33	-0.20	-26.48	-7.69	-9.19	-15.15
ϵ_{f+1}^n	4.25	2.38	1.89	-0.31	-2.00	-0.33	-8.48
$r_p^{(1)}$	1.669	1.718	1.732	2.089	2.103	2.190	2.319
β_p	0	0.06	0.06	0.23	0.42	0.53	0.59
γ_p	0	0	0	0	0	0	0
$r_n^{(1)}$	1.664	2.027	2.076	1.892	2.094	2.305	2.185
β_n	0	0.22	0.23	0.06	0.42	0.59	0.53
γ_n	0	0	0	0	0	0	0
$r_t^{(1)}$	1.667	1.909	1.946	1.953	2.098	2.256	2.263
β_t	0	0.17	0.18	0.18	0.42	0.56	0.57
γ_t	0	0	0	0	0	0	0
r_p	1.445	1.555	1.573	1.892	1.957	2.065	2.202
r_t	1.443	1.732	1.764	1.771	1.954	2.137	2.143
Q_o^p	0	0.004	0.004	0.059	0.083	0.103	0.173
P	0.0011				0.0053		

Table continued

^a $\hbar\omega$ is the frequency of the oscillator wavefunction. β and γ (in degrees) are the deformation parameters defined by the equation

$$\langle x_k^2 \rangle = \left[\prod_{i=1}^3 \langle x_i^2 \rangle \right]^{1/3} \exp \left\{ 2 \sqrt{\frac{5}{4\pi}} \beta \cos \left(\gamma - k \frac{2\pi}{3} \right) \right\}, k = 1, 2, 3.$$

β_o and γ_o are input data used in the code ELMOS [19] to generate the initial density matrix. $W \equiv W^{(2)}$ is the total binding energy as defined in Eq. (2.24b). W_c and $W_{c,D}$ are the total and direct Coulomb energies, respectively. ϵ_1 , ϵ_f and ϵ_{f+1} are the sp energies of the most deeply bound, last occupied and first unoccupied orbitals, respectively. $r^{(1)}$ is the sp rms radius. r is the rms radius with respect to the c.m. Q_o is the intrinsic proton quadrupole moment. The superscripts or subscripts p , n and t stand for proton, neutron and total, respectively. All energies are in units of MeV, all lengths are in units of Fermis and Q_o is in barns. P is the isospin impurity; see text.

TABLE II (continued)

	^8Be	^9Be	^9B	^{10}B	^{11}B	^{11}C	^{12}C
π_w	17.5	17.5	17.5	17.5	17.5	17.5	17.5
β_o	0.70	0.52	0.52	0.47	0.47	0.47	0.47
γ_o	0	5.0	5.0	35.0	170.0	170.0	180.0
$-W$	44.435	45.557	43.551	47.077	59.417	56.826	76.072
W_c	3.416	3.476	5.468	5.487	5.541	8.118	8.223
$W_{c,D}$	5.065	5.123	7.489	7.523	7.589	10.585	10.731
ϵ_1^p	-32.10	-37.30	-37.05	-41.80	-46.63	-42.24	-47.08
ϵ_f^p	-14.93	-15.90	- 1.89	- 9.57	-15.77	-10.17	-16.67
ϵ_{f+1}^p	0.48	- 3.59	- 0.29	- 4.14	-10.35	- 0.98	- 2.44
ϵ_1^n	-33.80	-39.52	-38.82	-44.09	-45.19	-48.77	-49.86
ϵ_f^n	-16.54	- 4.39	-17.55	-12.12	-12.75	-18.31	-19.25
ϵ_{f+1}^n	- 1.49	- 2.73	- 5.55	- 6.12	- 3.89	-12.32	- 5.36
$r_p^{(1)}$	2.340	2.292	2.389	2.369	2.339	2.399	2.367
β_p	0.67	0.62	0.44	0.47	0.46	0.44	0.46
γ_p	0	0.14	0.68	32.3	160.3	172.7	180.0
$r_n^{(1)}$	2.331	2.373	2.288	2.357	2.383	2.330	2.354
β_n	0.67	0.44	0.62	0.47	0.44	0.46	0.46
γ_n	0	0.58	0.16	32.3	172.7	160.2	180.0
$r_t^{(1)}$	2.336	2.338	2.345	2.363	2.363	2.368	2.361
β_t	0.67	0.52	0.52	0.47	0.45	0.45	0.46
γ_t	0	0.37	0.44	32.3	167.1	167.1	180.0
r_p	2.247	2.213	2.292	2.285	2.264	2.321	2.299
r_t	2.243	2.249	2.256	2.280	2.287	2.292	2.293
Q_o^p	0.200	0.178	0.180	0.145	- 0.126	- 0.161	- 0.162
P	0.0064			0.0220			0.0453

Table continued

TABLE II (continued)

	$^{12}\text{C}^*$	^{13}C	^{13}C	^{13}N	^{14}N	^{15}N	^{15}O
$\hbar\omega$	13.5	17.5	15.0	15.0	15.0	15.0	15.0
β_o	1.16	0.30	0.30	0.30	0.05	0.005	0.005
γ_o	0	180.0	180.0	180.0	180.0	180.0	180.0
$-W$	57.441	80.938	80.871	77.991	89.734	108.400	104.894
W_c	7.202	8.285	8.187	11.038	11.363	11.423	14.895
$W_{c,D}$	9.388	10.789	10.656	13.906	14.261	14.343	18.268
ϵ_1^p	-37.03	-51.25	-50.32	-51.99	-55.88	-58.83	-56.99
ϵ_f^p	-9.31	-17.98	-17.71	-7.99	-14.72	-17.49	-15.69
ϵ_{f+1}^p	-1.61	-7.83	-8.02	-3.33	-14.25	-17.15	3.66
ϵ_1^n	-39.49	-56.59	-55.58	-52.90	-59.30	-60.99	-61.97
ϵ_f^n	-11.60	-11.30	-11.45	-20.24	-18.21	-19.20	-20.63
ϵ_{f+1}^n	-4.27	-5.95	-6.22	-10.86	-17.27	0.39	-20.50
$r_p^{(1)}$	2.929	2.345	2.376	2.452	2.376	2.359	2.416
β_p	0.97	0.40	0.40	0.21	0.04	0.003	0.001
γ_p	0	180.0	180.0	180.0	180.0	180.0	180.0
$r_n^{(1)}$	2.920	2.395	2.431	2.365	2.359	2.395	2.347
β_n	0.97	0.22	0.21	0.40	0.04	0.001	0.003
γ_n	0	180.0	180.0	180.0	180.0	180.0	180.0
$r_t^{(1)}$	2.924	2.372	2.406	2.412	2.368	2.379	2.384
β_t	0.97	0.30	0.29	0.29	0.04	0.002	0.002
γ_t	0	180.0	180.0	180.0	180.0	180.0	180.0
r_p	2.815	2.284	2.314	2.381	2.313	2.303	2.357
r_t	2.870	2.307	2.340	2.346	2.306	2.321	2.327
Q_o^p	0.710	-0.142	-0.146	-0.108	-0.035	-0.000	-0.000
P					0.0386		

Table continued

TABLE II (continued)

	^{16}O	$^{16}\text{O}^{\#}$	^{17}O	^{17}F	^{18}F	^{19}F	^{19}Ne
$\hbar\omega$	15.0	13.5	15.0	15.0	15.0	15.0	15.0
β_{O}	0.001	0.83	0.10	0.10	0.25	0.35	0.35
γ_{O}	0	26.0	0	0	0	0	0
$-W$	125.704	92.962	126.303	122.838	125.758	135.751	131.828
W_{C}	14.987	13.098	14.889	18.323	18.152	18.060	21.960
$W_{\text{C,D}}$	18.390	16.072	18.271	22.100	21.922	21.828	26.157
$\epsilon_{\text{l}}^{\text{p}}$	-60.25	-47.70	-61.49	-60.87	-62.28	-64.15	-62.05
$\epsilon_{\text{f}}^{\text{p}}$	-17.64	-10.95	-19.40	0.43	- 5.52	-10.39	- 6.12
$\epsilon_{\text{f}+1}^{\text{p}}$	2.80	3.92	- 0.20	2.04	- 1.47	- 6.36	0.04
$\epsilon_{\text{l}}^{\text{n}}$	-64.09	-51.12	-65.20	-65.19	-66.51	-66.79	-68.23
$\epsilon_{\text{f}}^{\text{n}}$	-21.14	-13.95	- 3.32	-22.76	- 9.40	-10.03	-14.30
$\epsilon_{\text{f}+1}^{\text{n}}$	- 0.52	- 7.40	- 1.79	- 3.70	- 4.91	- 4.21	- 9.79
$r_{\text{p}}^{(1)}$	2.398	2.875	2.414	2.542	2.575	2.589	2.685
β_{p}	0	0.72	0.04	0.16	0.25	0.29	0.38
γ_{p}	0	24.8	0	0	0	0	0
$r_{\text{n}}^{(1)}$	2.381	2.857	2.518	2.399	2.555	2.662	2.572
β_{n}	0	0.72	0.16	0.04	0.25	0.38	0.29
γ_{n}	0	24.7	0	0	0	0	0
$r_{\text{t}}^{(1)}$	2.390	2.866	2.469	2.476	2.565	2.628	2.632
β_{t}	0	0.72	0.11	0.11	0.251	0.34	0.34
γ_{t}	0	24.8	0	0	0	0	0
r_{p}	2.345	2.826	2.364	2.490	2.527	2.544	2.640
r_{t}	2.337	2.818	2.419	2.426	2.518	2.584	2.588
Q_{O}^{p}	0	0.570	0.022	0.147	0.199	0.236	0.375
P	0.0461				0.0655		

Table continued

TABLE II (continued)

	^{20}Ne	^{21}Ne	^{21}Na	^{22}Na	^{23}Na	^{23}Mg	^{24}Mg
π_w	15.0	15.0	15.0	15.0	15.0	15.0	15.0
β_o	0.45	0.42	0.42	0.42	0.44	0.44	0.46
γ_o	0	1.0	1.0	1.0	15.0	15.0	20.0
$-W$	146.884	152.499	148.267	156.370	166.175	161.550	176.460
W_c	21.871	21.813	26.005	25.969	25.737	30.331	30.223
$W_{c,D}$	26.084	26.012	30.629	30.589	30.400	35.390	35.284
ϵ_l^p	-62.96	-64.45	-64.13	-65.35	-66.03	-64.36	-65.30
ϵ_f^p	-11.41	-12.68	- 2.45	- 4.18	- 9.82	- 6.95	-10.50
ϵ_{f+1}^p	- 1.38	- 3.80	- 1.71	- 3.68	- 7.26	- 1.09	- 1.99
ϵ_l^n	-67.55	-69.29	-68.85	-70.35	-69.85	-70.80	-70.61
ϵ_f^n	-15.32	- 7.06	-16.62	- 8.40	-11.54	-14.45	-15.12
ϵ_{f+1}^n	- 5.60	- 5.93	- 8.03	- 8.29	- 5.97	-11.46	- 6.88
$r_p^{(1)}$	2.701	2.708	2.778	2.782	2.808	2.864	2.874
β_p	0.42	0.42	0.41	0.42	0.44	0.45	0.46
γ_p	0	0.01	0.03	0.4	14.2	18.6	21.2
$r_n^{(1)}$	2.681	2.754	2.691	2.761	2.840	2.790	2.853
β_n	0.42	0.42	0.42	0.42	0.45	0.44	0.46
γ_n	0	0.02	0.01	0.4	18.6	14.2	21.1
$r_t^{(1)}$	2.691	2.732	2.736	2.772	2.825	2.829	2.864
β_t	0.42	0.42	0.42	0.42	0.44	0.44	0.46
γ_t	0	0.02	0.02	0.4	16.5	16.6	21.2
r_p	2.660	2.670	2.738	2.745	2.773	2.828	2.841
r_t	2.650	2.694	2.698	2.735	2.790	2.794	2.831
Q_o^p	0.420	0.427	0.484	0.493	0.488	0.563	0.573
P	0.0725			0.0897			0.0990

Table continued

TABLE II (continued)

	^{25}Mg	^{25}Al	^{26}Al	^{27}Al	^{27}Si	^{28}Si	^{29}Si
$\pi\omega$	15.0	15.0	15.0	15.0	15.0	15.0	15.0
β_{O}	0.44	0.44	0.45	0.45	0.45	0.48	0.45
γ_{O}	30.0	30.0	45.0	173.0	173.0	180.0	177.0
$-W$	181.029	176.225	184.708	198.846	193.502	212.366	218.744
W_{C}	30.173	34.927	34.894	34.872	40.164	40.126	40.061
$W_{\text{C,D}}$	35.215	40.391	40.355	40.337	46.066	46.042	45.958
$\epsilon_{\text{l}}^{\text{P}}$	-66.96	-66.42	-67.96	-70.00	-67.76	-69.33	-70.78
$\epsilon_{\text{f}}^{\text{P}}$	-11.72	- 3.59	- 8.19	-12.67	- 9.18	-13.28	-13.40
$\epsilon_{\text{f+l}}^{\text{P}}$	- 4.04	- 1.72	- 4.67	- 9.35	- 1.01	- 1.23	- 4.08
$\epsilon_{\text{l}}^{\text{n}}$	-72.28	-72.10	-73.68	-73.99	-75.57	-75.42	-77.30
$\epsilon_{\text{f}}^{\text{n}}$	- 8.88	-16.32	-13.48	-14.51	-17.97	-18.62	- 9.71
$\epsilon_{\text{f+l}}^{\text{n}}$	- 6.87	- 8.84	- 9.51	- 6.54	-14.19	- 6.77	- 7.17
$r_{\text{p}}^{(1)}$	2.874	2.932	2.931	2.930	2.974	2.978	2.980
β_{p}	0.45	0.44	0.44	0.45	0.46	0.47	0.46
γ_{p}	25.8	37.7	43.1	168.3	176.0	180.0	178.2
$r_{\text{n}}^{(1)}$	2.906	2.855	2.908	2.949	2.910	2.955	2.994
β_{n}	0.44	0.45	0.44	0.46	0.45	0.47	0.41
γ_{n}	37.7	25.6	43.0	176.0	168.1	180.0	174.0
$r_{\text{t}}^{(1)}$	2.891	2.895	2.920	2.940	2.943	2.966	2.987
β_{t}	0.44	0.44	0.44	0.45	0.45	0.47	0.48
γ_{t}	32.1	32.0	43.1	172.4	172.4	180.0	176.2
r_{p}	2.842	2.898	2.900	2.900	2.944	2.949	2.953
r_{t}	2.859	2.863	2.889	2.910	2.913	2.938	2.960
Q_{O}^{P}	0.536	0.493	0.588	- 0.520	- 0.596	- 0.611	- 0.597
P			0.1292			0.1373	

Table continued

TABLE II (continued)

	^{29}Si	^{29}P	^{30}P	^{31}P	^{31}S	^{32}S	^{33}S
$\hbar\omega$	13.5	13.5	13.5	13.5	13.5	13.5	13.5
β_0	0.45	0.45	0.40	0.35	0.35	0.35	0.30
γ_0	177.0	177.0	172.0	167.0	167.0	161.0	165.0
$-W$	218.539	213.096	222.706	236.032	230.156	246.823	255.707
W_c	39.690	45.046	45.007	44.993	50.804	50.777	50.850
$W_{c,D}$	45.916	51.191	51.254	51.244	57.495	57.482	57.546
ϵ_l^p	-70.06	-69.91	-70.69	-72.33	-70.44	-71.24	-72.99
ϵ_f^p	-13.40	- 3.95	- 7.15	-10.31	- 7.66	-10.82	-11.53
ϵ_{f+1}^p	- 4.20	- 1.70	- 4.67	- 7.90	- 2.10	- 2.87	- 5.82
ϵ_l^n	-76.54	-75.92	-77.13	-77.41	-78.57	-78.01	-80.19
ϵ_f^n	- 9.80	-18.64	-13.01	-13.52	-16.17	-16.68	-12.07
ϵ_{f+1}^n	- 7.34	- 9.63	-10.11	- 8.22	-13.34	- 8.98	- 9.47
$r_p^{(1)}$	3.014	3.058	3.059	3.058	3.094	3.094	3.086
β_p	0.46	0.41	0.40	0.39	0.36	0.36	0.34
γ_p	178.3	174.0	171.5	169.0	164.0	161.0	162.7
$r_n^{(1)}$	3.027	2.989	3.030	3.061	3.032	3.064	3.087
β_n	0.41	0.46	0.40	0.36	0.39	0.36	0.30
γ_n	174.0	178.3	171.5	163.9	169.0	160.9	165.9
$r_t^{(1)}$	3.020	3.025	3.017	3.060	3.064	3.079	3.087
β_t	0.44	0.44	0.40	0.38	0.38	0.36	0.32
γ_t	176.2	176.2	171.5	166.5	166.5	161.0	164.2
r_p	2.985	3.029	3.031	3.031	3.067	3.068	3.061
r_t	2.992	2.997	3.017	3.033	3.038	3.054	3.062
Q_o^p	- 0.616	- 0.617	- 0.603	- 0.590	- 0.590	- 0.578	- 0.554
P			0.2525			0.2260	

Table continued

TABLE II (continued)

	^{33}Cl	^{34}Cl	^{35}Cl	^{35}Ar	^{36}Ar	^{37}Ar	^{37}K
$\hbar\omega$	13.5	13.5	13.5	13.5	13.5	13.5	13.5
β_0	0.30	0.28	0.25	0.25	0.25	0.15	0.15
γ_0	165.0	170.0	175.0	175.0	180.0	180.0	180.0
$-W$	249.584	261.436	276.955	270.379	288.978	298.298	291.534
W_C	56.873	56.948	57.045	63.538	63.618	63.699	70.353
$W_{C,D}$	64.002	64.078	64.177	71.121	71.214	71.287	78.373
ϵ_1^p	-72.80	-73.88	-75.73	-73.91	-75.00	-76.91	-76.64
ϵ_f^p	- 5.53	- 8.54	-11.47	- 9.08	-11.78	-12.88	- 6.50
ϵ_{f+1}^p	- 3.33	- 6.20	- 9.36	- 1.29	- 2.67	- 6.28	- 3.44
ϵ_1^n	-79.58	-81.06	-81.65	-82.72	-82.55	-84.80	-84.27
ϵ_f^n	-17.40	-15.13	-15.65	-18.00	-18.34	-13.72	-19.44
ϵ_{f+1}^n	-11.93	-12.33	- 8.01	-15.50	- 9.41	-10.24	-13.43
$r_p^{(1)}$	3.122	3.114	3.106	3.135	3.129	3.121	3.155
β_p	0.30	0.29	0.27	0.25	0.24	0.20	0.14
γ_p	165.9	168.5	171.6	176.0	180.0	180.0	180.0
$r_n^{(1)}$	3.059	3.083	3.100	3.077	3.097	3.119	3.091
β_n	0.34	0.29	0.25	0.27	0.24	0.14	0.20
γ_n	162.6	168.5	176.1	171.5	180.0	180.0	180.0
$r_t^{(1)}$	3.091	3.099	3.103	3.107	3.113	3.120	3.124
β_t	0.32	0.29	0.26	0.26	0.24	0.17	0.17
γ_t	164.2	168.5	173.8	173.7	180.0	180.0	180.0
r_p	3.096	3.090	3.082	3.111	3.106	3.098	3.132
r_t	3.066	3.074	3.079	3.084	3.090	3.098	3.102
Q_O^p	- 0.551	- 0.528	- 0.505	- 0.502	- 0.482	- 0.420	- 0.314
P		0.2628			0.4033		

Table continued

TABLE II (continued)

	^{38}K	^{39}K	^{39}Ca	^{40}Ca	^{41}Ca	^{41}Sc
$\pi\omega$	13.5	13.5	13.5	13.5	13.5	13.5
β_o	0.10	0.04	0.04	0.01	0.04	0.04
γ_o	180.0	180.0	180.0	180.0	180.0	180.0
-W	304.736	324.300	317.048	337.812	340.898	333.467
W_c	70.455	70.653	77.795	77.934	77.722	85.060
$W_{c,D}$	78.477	78.670	96.278	86.322	86.142	94.003
ϵ_1^p	-77.83	-79.29	-77.73	-79.25	-79.97	-79.31
ϵ_f^p	-10.39	-13.17	-11.57	-13.89	-13.79	4.15
ϵ_{f+1}^p	- 7.12	-12.57	4.74	4.71	2.12	4.26
ϵ_1^n	-85.81	-86.26	-87.08	-87.58	-88.06	-88.20
ϵ_f^n	-17.60	-18.87	-20.04	-21.15	- 3.52	-21.04
ϵ_{f+1}^n	-13.92	- 2.67	-19.40	- 2.74	- 3.31	- 5.32
$r_p^{(1)}$	3.148	3.137	3.167	3.165	3.171	3.202
β_p	0.11	0.06	0.02	0	0.01	0.04
γ_p	180.0	180.0	180.0	0	180.0	180.0
$r_n^{(1)}$	3.114	3.130	3.106	3.131	3.168	3.138
β_n	0.11	0.02	0.06	0	0.05	0.01
γ_n	180.0	180.0	180.0	0	180.0	180.0
$r_t^{(1)}$	3.131	3.134	3.138	3.148	3.170	3.171
β_t	0.11	0.04	0.04	0	0.03	0.03
γ_t	180.0	180.0	180.0	0	180.0	180.0
r_p	3.126	3.116	3.145	3.144	3.151	3.181
r_t	3.109	3.112	3.116	3.127	3.149	3.151
Q_o^p	- 0.244	- 0.146	- 0.050	0	- 0.039	- 0.121
P	0.3348			0.3687		

of the c.m. from the Hamiltonian *before* the iterations and by computing radii *with respect to* the c.m. (see Subsection 2.E for further details). The Coulomb two-body interaction is contained in our Hamiltonian, and its matrix elements, together with those of other central two-body operators, were conveniently computed exactly using Talman's method [23].

It is clear that only a fraction of the large amount of information made available by this type of microscopic calculation can be reported here. The master Table II and Section III present some of those, such as ground state binding energies (3.B), separation energies and Fermi energies (3.C), density distributions and alpha clusters (3.D), rms radii (3.E) and their differences (3.G), intrinsic quadrupole moments (3.F), Coulomb energies (3.H) and Isospin impurities (3.I). The last three sections make new predictions about these effects. The matter of HF single-particle energies is discussed in Section 2.F. The experimental interpretation of these results is problematic so that no details concerning these will be given at this time.

Additional numerical information may be obtained by using the computer code EVALIN, written in CDC 6600 FORTRAN IV language, copies of which are available as an AECL report [24]. This code was used to obtain the results reported here.

2. METHOD OF CALCULATION

A. The Hartree-Fock Approximation

The Hartree-Fock method has been well reviewed [25] in the past so that only a brief description of its derivation will be given here. The antisymmetrized ground-state wavefunction of the A -Fermion nuclear system is to be approximated by an "optimal" SD $|\Psi_0\rangle$, which we write, in second quantization notation, as

$$|\Psi_0\rangle = \prod_{i=1}^A \xi_i^\dagger |0\rangle, \quad (2.1)$$

where $|0\rangle$ is the vacuum state, and $\xi_i^\dagger(\xi_i)$, $i = 1, \dots, A$ are the creation (annihilation) operators for the single-particle (sp) occupied states. We use the subscripts i, j for occupied sp states, m, n for unoccupied states and k, l, r, s , for either kind. Thouless [26] has shown that any other SD , $|\Psi\rangle$, which is independent of $|\Psi_0\rangle$ can be written as

$$|\Psi(Z)\rangle = \exp\left(\sum_{m,i} Z_{mi} \xi_m^\dagger \xi_i\right) |\Psi_0\rangle, \quad (2.2)$$

and that the energy minimisation condition

$$\lim_{Z \rightarrow 0} \frac{\partial}{\partial Z_{mi}} W(Z) = \lim_{Z \rightarrow 0} \frac{\partial}{\partial Z_{mi}} \frac{\langle \Psi(Z) | H | \Psi(Z) \rangle}{\langle \Psi(Z) | \Psi(Z) \rangle} = 0 \quad (2.3)$$

leads to

$$\langle \Psi_0 | H \xi_m^\dagger \xi_i | \Psi_0 \rangle = 0, \quad \text{all } i, m, \quad (2.4)$$

where H is the Hamiltonian of the system, provided that a stability condition [26, 27] is met. This last equation is the fundamental defining equation of the HF state $|\Psi_0\rangle$. In particular, it does not imply that $|\Psi_0\rangle$ should be an eigenstate of any of the operators which commute with H .

The HF single-particle energies are next defined as

$$\langle \Psi_0 | [H, \xi_i^\dagger] \xi_j | \Psi_0 \rangle = \epsilon_i \delta_{ij}, \quad (2.5a)$$

and

$$\langle \Psi_0 | \xi_n [H, \xi_m^\dagger] | \Psi_0 \rangle = \epsilon_m \delta_{mn}. \quad (2.5b)$$

We let the Hamiltonian be composed of a one-body part T (the kinetic energy) and a two-body part v , so that

$$H = \sum_{kl} T_{kl} \xi_k^\dagger \xi_l + \frac{1}{4} \sum_{klrs} v_{klrs} \xi_k^\dagger \xi_l^\dagger \xi_r \xi_s, \quad (2.6)$$

where v_{klrs} are the antisymmetrised two-body matrix elements of v . This reduces the Eqs. (2.4) and (2.5) to

$$T_{kl} + \sum_i v_{kili} = \epsilon_k \delta_{kl}, \quad (2.7)$$

and yields the expression for W :

$$W = \langle \Psi_0 | H | \Psi_0 \rangle = \sum_i T_{ii} + \frac{1}{2} \sum_{ij} v_{ijij} = \frac{1}{2} \sum_i (\epsilon_i + T_{ii}).$$

The solution of Eq. (2.7) is carried out by expanding $\xi_i^\dagger$ as linear combinations of the basis creation operators [28] $a_\alpha^\dagger$, as follows;

$$\xi_i = \sum_\alpha a_\alpha u_{\alpha i}^*, \quad \xi_i^\dagger = (\xi_i)^\dagger, \quad (2.8)$$

where $u_{\alpha i}$ is the required complex unitary transformation matrix and constitutes the set of sp “wavefunctions” of the HF orbitals. The details of the phase con-

ventions in the expansion basis are not required here but are important for computational purposes. They are given in Ref. [24]. Equation (2.7) now becomes an explicit eigenvalue equation

$$\sum_{\beta} (T_{\alpha\beta} + U_{\alpha\beta}) u_{\beta l} = u_{\alpha l} \epsilon_l, \quad (2.9)$$

where $U_{\alpha\beta}$ is the HF sp average potential matrix,

$$U_{\alpha\beta} = \sum_{\gamma\delta} v_{\alpha\gamma\beta\delta} \rho_{\delta\gamma}, \quad (2.10)$$

and is defined through the *average* of the one-body density matrix operator,

$$\rho_{\delta\gamma} = \langle \Psi_0 | a_{\gamma}^{\dagger} a_{\delta} | \Psi_0 \rangle = \sum_i u_{\delta i} u_{\gamma i}^*. \quad (2.11)$$

By definition, ρ is hermitian; the unitarity of $u_{\alpha\beta}$ ensures that $\rho^2 = \rho$.

$$W = \sum_{\alpha\beta} (T_{\alpha\beta} + \frac{1}{2} U_{\alpha\beta}) \rho_{\beta\alpha} = \text{Tr}[\mathbf{T}\rho + \frac{1}{2} \mathbf{U}\rho] = \frac{1}{2} \sum_i \epsilon_i + \frac{1}{2} \text{Tr}[\mathbf{T}\rho], \quad (2.12)$$

where we have made use of Eq. (2.9) for the last step. The sequence Eqs. (2.11), (2.10) and (2.9) represents the basic iteration loop. The initial values of $u_{\alpha i}$ are taken as Nilsson model wavefunction expansion coefficients [19], including nonaxiality and major oscillator shell mixing. The selection of the occupied states in the initial wavefunction is made by choosing those Nilsson orbits which have the lowest energy. The initialisation will be described in more detail in Subsection 2-H. The density matrix and the sp potential are then computed and the diagonalisation, Eq. (2.9), is performed. After each iteration the new set of occupied orbits is taken to be the one with the lowest current values of ϵ_i . In practice the rate of convergence to a stable $u_{\alpha k}$ depends on several factors such as the structure of the twobody potential matrix elements $v_{\alpha\beta\gamma\delta}$, the choice of the model parameters for the initial wavefunction, the dimension of the expansion basis, and the energy difference between the highest occupied state and the lowest unoccupied state (energy gap). It may happen that the iterations fail to converge altogether but instead oscillate back and forth between two or more sets of $u_{\alpha k}$'s. This behavior occurs more often when a small expansion basis is selected so that the number of degrees of freedom is reduced [29]. With the large basis used here and a careful choice of $u_{\alpha i}^{(0)}$ we have been able to find stable solutions for all the nuclei studied, although in the worst case (^{23}Mg in Table II) 12 iterations were required instead of the usual 6. The remainder of Section 2 will be devoted to specific points of interest in the calculation.

B. The Expansion Basis and the Representation Convention

The expansion basis states are taken to be those of the $sp\ j-j$ coupled spherical harmonic oscillator for a spin $\frac{1}{2}$ particle. The truncation is dictated by practical considerations. The largest basis discussed here includes the first five major oscillator shells plus the $0h_{11/2}$ orbit of the $N = 5$ shell and its structure is given in Table I. It can, in principle, accommodate up to 82 protons and 82 neutrons so that no more than $\frac{1}{4}$ of it is ever occupied by the nuclei of interest here ($A \lesssim 40$). It is known that the size of the basis has important effects on the quadrupole [8, 30] and higher multipole moments, provided only a fraction of it is occupied. A large basis will also allow the proton distribution to expand, due to the repulsive Coulomb force, beyond that of the corresponding neutrons.

In a computation of the present magnitude it is essential to minimize the computing time for the basic iteration loop of Subsection A. Whereas the matrix diagonalization implied by Eq. (2.9) requires an algorithm which is a cubic function of the basis dimension, the construction of $U_{\alpha\beta}$ in Eq. (2.10) is a *quartic* process. Using only the antisymmetry relations [31] on $v_{\alpha\beta\gamma\delta}$, we could have as many as $(82)^4/2^3 \approx 6 \times 10^6$ distinct matrix elements of v . In fact, the rotational invariance of v implies that there are fewer than 1.5×10^4 distinct reduced matrix elements. This factor of 500 can be utilized with advantage even though we are *not* restricting ourselves to spherical HF calculations. We first state the notation convention [32] and use it to describe a method we believe to be new for computing deformed potentials using only reduced matrix elements.

We let α be a set of quantum numbers necessary to define a sp state, apart from the isospin labels, and a be the same set minus the magnetic quantum number m_a ; that is

$$\alpha \equiv (n_a, l_a, j_a, m_a, \text{etc}) \equiv (a, m_a).$$

We also put

$$\bar{\alpha} \equiv (a, -m_a); \quad s_a \equiv (-1)^{j_a - m_a},$$

and

$$C_{\alpha\beta}^{JM} \equiv \langle j_a, j_b, m_a, M - m_a | JM \rangle;$$

the last equation gives us a short-hand notation for the usual Clebsch-Gordan coefficient. Using a slight variation of Baranger's [31] notation we define the G and F reduced matrix elements of v through the equations

$$v_{\alpha\beta\gamma\delta} = \sum_J C_{\alpha\beta}^{JM} C_{\gamma\delta}^{JM} G_{abcd}^J = \sum_J C_{\alpha\bar{\gamma}}^{JM} s_\gamma C_{\delta\bar{\beta}}^{JM} s_\beta F_{acdb}^J. \quad (2.13)$$

Here we pursue this kind of expansion further and write

$$U_{ab}^{JK} = \sum_{m_a m_b} C_{\alpha\beta}^{JK} s_\beta U_{\alpha\beta}. \quad (2.14)$$

The quantities U_{ab}^{JK} are akin to “reduced matrix elements” of the deformed HF sp potential $U_{\alpha\beta}$. Equation (2.14) may be applied to $\rho_{\alpha\beta}$ and to the other sp operators. The number of such reduced matrix elements is similar to the original number of $U_{\alpha\beta}$, and the relevant selection rules and symmetries remain simple to apply. For example, the hermiticity of $\rho_{\alpha\beta}$ yields

$$\rho_{dc}^{J,-K} = (-1)^{M+j_d-j_c} \rho_{cd}^{JK*}. \quad (2.15)$$

Thus only components of ρ with $K \geq 0$ need be calculated. It will be noticed that these reduced matrix elements do depend on K , the angular momentum projection along the intrinsic z axis; this effect is well known to occur whenever one deals with a deformed intrinsic state [33]. The expression (2.14) leads to interesting angular momentum expansions for the total binding energy W , but space limitations preclude a discussion of these results here. The most important result of Eq. (2.14), however, is the new equation

$$U_{ab}^{JK} = \sum_{dc} F_{abca}^J \rho_{cd}^{JK}, \quad (2.16)$$

which may be used instead of Eq. (2.10), resulting in a very much faster computation of the sp field.

C. Matrix Elements of the Coulomb and other central Two-Body Operators

The Coulomb two-body interaction is to be included in the total Hamiltonian so that its F -matrix elements must be obtained. When computing the kinetic energy and mean-square radius with respect to the c.m., the two-body matrix elements of $|p_1 - p_2|^2$ and $|r_1 - r_2|^2$ will also be needed. The long-range nature of these operators results in a poorly convergent infinite partial wave expansion in the Talmi-Moshinsky scheme used to compute the matrix element of v . However, we have found that the closed form method developed recently by Talman [23] is fast and numerically stable for this purpose.

A general antisymmetrised F matrix element can be written as

$$F_{abcd}^J = f_{abcd}^J - (-1)^{j_a+j_d+J} \sum_{J'} (2J' + 1)(-1)^{J'} W(j_a j_b j_c j_d; JJ') f_{acbd}^{J'}. \quad (2.17)$$

The direct matrix element f_{abcd}^J of a central operator is obtained, following Talman, as

$$\begin{aligned} f_{abcd}^J = & c_a c_b c_c c_d (-1)^{j_a-j_c+(l_b+l_c-l_a-l_d)/2} \\ & \times \frac{\hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d}{(2J+1)} W(l_a l_b j_a j_b; J_{\frac{1}{2}}) W(l_c l_d j_c j_d; J_{\frac{1}{2}}) \sum_{NM\nu} \mathcal{C}_{NJ}^{ab} \mathcal{C}_{MJ}^{cd} \mathcal{R}(NMJ\nu) I_\nu, \end{aligned} \quad (2.18)$$

where $j \equiv \sqrt{2j+1}$, and the angular momentum phase factors in (2.18) reflects our use of the Wigner time-reversal phase convention [35] throughout. The coefficients c_a , $\mathcal{C}_{NJ}^{ab}$, $\mathcal{R}(NMJ\nu)$ are given by Talman [23] in his Eqs. (4), (14) and (15). The symbol W is the usual Racah coefficient [32] and I_ν represents the Talmi integral

$$I_\nu = 4\pi \int_0^\infty r^{2\nu+2} e^{-r^2} v(\sqrt{2} r) dr, \quad (2.19)$$

which takes the values $e^2\pi\nu!/\sqrt{2}$ for the Coulomb potential $v_c = e^2/r$. Our discussion has so far neglected the isospin quantum numbers. As we shall see in the following subsections, we have elected to treat neutrons and protons separately. It can be shown that for our purpose this only implies that certain matrix elements F in Eq. (2.17) should be computed *without* including the exchange term. The isospin analysis for the nuclear part of the potential is carried out in the next subsection.

D. Isospin Components of the F Matrix Elements of V

Primarily because of the presence of the Coulomb part of H it is more convenient to compute and treat separately the various operators in terms of their proton and neutron components. Subsection H will outline the resulting breakup of the basic Eqs. (2.9–11) in terms of the various components of F which we describe here.

We let τ_a be the isospin projection component of state α and we consider the isospin reduction analogous to Eq. (2.13), namely,

$$F_{\tau_a, \tau_b, \tau_c, \tau_d}^J = \sum_T C_{\tau_a \tau_b}^{T\tau} C_{\tau_c \tau_d}^{T\tau} F_{abcd}^{JT}, \quad (2.20)$$

where T and τ are the two-particle isospin and projection, respectively, and F_{abcd}^{JT} is related to the more familiar G^{JT} matrix element by

$$F_{abcd}^{JT} = -\frac{1}{2} \sum_{J'} (2J' + 1) W(adb c; J' J) [G_{adb c}^{J'0} (\delta_{T,1} - \delta_{T,0}) + G_{adb c}^{J'1} (\delta_{T,1} + 3\delta_{T,0})]. \quad (2.21)$$

Omitting J and the other labels, this general expression gives

$$F_{pp} \equiv F_{pp,pp} = \frac{1}{2}(F^0 + F^1) + F_c, \quad (2.22a)$$

$$F_{pn} \equiv F_{pp,nn} = F_{nn,pp} = \frac{1}{2}(F^0 - F^1), \quad (2.22b)$$

$$F_{nn} \equiv F_{nn,nn} = \frac{1}{2}(F^0 + F^1), \quad (2.22c)$$

$$F_{pn,pn} = F_{np,np} = F^1. \quad (2.22d)$$

The overall effects of F^0 and F^1 may be estimated by computing the ratio E_{pn}/E_{nn}

of the potential energy due to F_{pn} and to F_{nn} . For ^{16}O , ^{28}Si and ^{40}Ca we have found the values 2.16, 1.95 and 1.94, respectively. This implies $F^0 \approx -3F^1$ and shows that F^1 is repulsive and approximately thrice as weak as F^0 . This fact is usually taken as justification for neglecting $F_{pn,pn}$, the charge-exchange term in Eq. (2.22d), in HF iterations since the weak and repulsive nature of F^1 is not expected to induce neutron-proton mixing in the sp HF orbitals. Furthermore, in the absence of such mixing the charge-exchange interaction fails to contribute to W , the total energy expectation value. We note that although F^1 does not appear to produce permanent "charge-exchange deformations" it is known to induce vibrations of the charge distribution. These are the coherent giant dipole [36] $T = 1$ states which are pushed *up* (because F^1 is repulsive) in the energy continuum. This is to be contrasted with the case of spatial quadrupole vibration which are generated by *attractive* interactions such that the energy of the vibrating state is pulled *down* towards the ground state.

We have followed the universal trend and ignored $F_{pn,pn}$ in the present HF calculation. However, we do not feel that the arguments for doing so are particularly strong especially when the further refinement of a Hill-Wheeler type projection is incorporated, and calculations which allow proton-neutron mixing should be performed in the future. They entail the introduction of a Lagrange multiplier to maintain the average value of $(N - Z)/2$. Furthermore, to take most advantage of this new variational degree of freedom, additional studies on the types of initial trial wave functions to be used should be made.

E. The c.m. Kinetic Energy and the Single-Particle Energies

Most of the initial trial wavefunctions used here have the property that their c.m. wavefunction resembles closely that of a 0s harmonic oscillator state. If we iterate these wavefunctions using the full Hamiltonian H , which contains the kinetic energy of the c.m., the final wavefunction will attempt to minimize also the kinetic energy of the c.m. and can only do so by delocalising the c.m., within the basis limitation. This effect destroys the interpretation of the sp wavefunction as being the wavefunction with respect to a fixed center and is usually discussed as the spurious c.m. motion [22] problem. We avoid it by conducting the iterations using the Hamiltonian with respect to the c.m. $H_{\text{rel}} = T_{\text{rel}} + V$, where

$$T_{\text{rel}} = \frac{1}{2m} \sum_{n=1}^A |\mathbf{p}_n - \mathbf{P}|^2 = \frac{1}{4mA} \sum_{nn'=1}^A |\mathbf{p}_n - \mathbf{p}_{n'}|^2, \quad (2.23)$$

is the kinetic energy with respect to the c.m. and $\mathbf{P} = 1/A \sum_{n=1}^A \mathbf{p}_n$, is the momentum of the c.m. The matrix elements of T_{rel} are obtained as in subsection C, and it is seen that H_{rel} no longer contains any one-body components but its matrix elements become *atomic number* dependent (e.g., the factor $1/A$ in Eq. 2.23).

We have found that the expansion basis used here is still too small to allow much delocalization of the c.m. so that the wavefunctions obtained by using either H or H_{rel} were similar. Thus we shall, from now on, consider only the wavefunctions $|\Psi_0\rangle$ and density matrices ρ obtained by using H_{rel} . We may compute the sp and total energy from Eqs. (2.5a) and (2.12) using both Hamiltonians, as

$$\epsilon_{i,\text{rel}} = \langle \Psi_0 | [H_{\text{rel}}, \xi_i^\dagger] \xi_i | \Psi_0 \rangle, \quad (2.24a)$$

$$W_{\text{rel}} = \frac{1}{2} \sum_i \epsilon_{i,\text{rel}}, \quad (2.24b)$$

$$\epsilon_i = \langle \Psi_0 | [H, \xi_i^\dagger] \xi_i | \Psi_0 \rangle, \quad (2.25a)$$

$$W = \frac{1}{2} \sum_i \epsilon_i + \frac{1}{2} \text{Tr}[\mathbf{T}\rho]. \quad (2.25b)$$

Actually W and W_{rel} differ only by the zero-point kinetic energy of the c.m., that is about $\frac{3}{4}\hbar\omega \sim 10\text{--}15$ MeV, in this case. Assuming $W_{\text{rel}} \approx W$ and recalling that T is a positive definite operator, we see that Eqs. (2.24b) and (2.25b) imply $\epsilon_{i,\text{rel}} > \epsilon_i$. Indeed we have observed that $\epsilon_{i,\text{rel}}$ is sometimes positive for some bound occupied orbitals near the Fermi sea. In fact, the definition of sp energies as observables is still the subject of some controversy [37]. Here we shall consider them only in the context of sp separation energies and use a theorem of Hugenholtz and Van Hove [38] whereby

$$\epsilon_{i,\text{sep}} = \frac{\langle \delta H \rangle}{\delta \rho_i} = \epsilon_i, \quad (2.26)$$

in the limit $A \rightarrow \infty$, for an interacting Fermi gas; here ρ_i should be the density matrix obtained by iterating with H , the total Hamiltonian. We shall from now on refer to the sp energies as those computed using (2.25a) and to the total energy as computed using (2.24b). The use of theorem (2.26) for finite nuclei is restricted to the computation of the separation energy of the last occupied orbit because of the large rearrangement energy of the other orbits. These Fermi energies are given in Subsection 3-C. The sp energy results for the other orbits will not be presented in detail here, except for $\epsilon_{0s1/2}$ in Table II, because of the ambiguities mentioned above. We only sketch here part of their systematics.

The systematic trend of the sp energies of the *occupied* states is generally in good qualitative agreement with those of the Nilsson model code ELMOS [19]. The most obvious quantitative disagreement is a wider shell gap for the HF sp energies than for the Nilsson sp energies. The values of the spin-orbit splittings of the occupied states are generally good. However the sp energies of the unoccupied states bear little resemblance to those of the Nilsson orbits where, as we said, no

systematically large gap above the Fermi sea is present. Most of the *sp* energies of unoccupied states appear to be randomly distributed in the “continuum”, up to about +60 MeV, and their corresponding *sp* wavefunctions have generally poor overlap with any one Nilsson orbit. This is in contrast with the occupied *sp* wavefunctions which generally have overlap of 0.90–0.95 with their corresponding Nilsson orbit.

F. Selection of the Two-Body Interaction

It was pointed out in the Introduction that the two-body interaction which is appropriate for HF calculations should be a Brueckner type energy dependent *K* matrix rather than a true potential which would fit the two-nucleon data. The results reported here were calculated using version No. (SP2) of the semi-realistic *N*–*N* potentials of Saunier and Pearson [14, 39]. These authors produced four versions of their interaction; here we discuss their method only briefly, in relation with SP2 and SP3.

These potentials are composed of a momentum-dependent, phenomenological short-range part which is matched at about one Fermi to a cutoff version of the long-range, static, one-boson-exchange potential of Bryan and Scott [40]. The parameters of SP3 were adjusted to give the best fit to the two-nucleon data and should therefore behave like a true potential. We have found that this potential did indeed yield HF results in rather good agreement with those obtained [9, 10] using the Tabakin potential. The parameters of SP2, on the other hand, were obtained by modifying those of SP3 in the singlet-even *N*–*N* scattering channel in order to obtain a good *first-order* HF fit to nuclear matter properties insofar as they are known. Since this is a criterion for a *K* matrix, SP2 should also give good HF results for finite nuclei provided the energy and density dependence of *K* is weak. To first order in nuclear matter, SP2 predicts 16 MeV per nucleon of binding energy at a saturation density corresponding to a Fermi momentum of $1.35 F^{-1}$ (a density of 0.166 nucleons/ F^3), a symmetry energy of 41.5 MeV and a compressibility of 256 MeV.

We have compared the results obtained by using SP2 with those obtained using the *K* matrices derived from other realistic interactions, namely the *K* matrix of the nonlocal separable potential of Kahana, Lee and Scott [41] (KLS), and the one derived by Shakin, Waghmare and Hull [42] from the Yale (1962) potential [43]. This last one was used in a three-major shell calculation by Pal and Stamp [7] (PS) and we shall quote their results in that basis (*N* = 0, 1, 2). The KLS interaction is also suitable for use in that basis, and for *A* ~ 16–20. In both cases the energy denominators used in the computation of *K* are reasonable but not self-consistent. The results for the binding energy of ^{16}O are 109.6, 108.4 and 120.4 MeV, using the KLS, PS, and SP2 (*N* = 0, 1, 2) interactions, and similarly 135.2, 132.2 and 134.9 MeV for ^{20}Ne (prolate). The results are remarkably similar

especially for ^{20}Ne , and support our assumption that SP2 is effectively a useful K matrix.

A true K matrix would yield binding energies which are independent of the basis dimension. The SP2 interaction was tested for this property by varying the number of major shells used. The maximum size of five major shells yielded the binding energies 125.7 and 146.6 MeV for ^{16}O and ^{20}Ne , respectively. The stronger basis dependence for ^{20}Ne is probably related to the fairly large deformation parameter ($\beta = 0.45$) of that nucleus which requires more major shell mixing in a spherical expansion basis.

G. Symmetries of the SP Density Matrix and Distributions

It was pointed out in Subsection 2.A that the HF equations do not imply that $|\Psi_0\rangle$ should be an eigenfunction of any of the operators which commute with H . In particular H and H_{rel} are invariant under the group of rotations R , the parity P and the time-reversal operator T . Thus, according to Eq. (2.10), the HF potential U has the same transformation properties under R, P, T as the density matrix ρ obtained from $|\Psi\rangle$. It then follows that the final HF solution cannot violate any symmetry which was included in trial density $\rho^{(0)}$. The only two symmetries of H which we shall conserve throughout are the isospin projection (no mixing of neutron and proton orbitals) and parity. The reasons for maintaining the first symmetry were discussed in Subsection 2.D. The reasons for conserving parity in the sp orbits are more involved. To begin with, a calculation which allows for parity mixing must provide initial density distributions which violate parity in a way which is fairly close to the desired final result, lest one find only a local minimum instead of an absolute minimum. Another possible outcome is that the solution will revert back to a parity conserving one if the initial density distribution is too far from the desired result. We have performed rather extensive parity violating calculations in a four major shell basis and have observed both these effects. Other authors have also failed to observe parity violation in the ground state [44]. Yet recent cluster model variational calculations [16, 17] claim that such violations can occur when alpha-particle cluster trial wavefunctions are used. We believe that careful studies of the energies of the projected states obtained from these wavefunctions will be required to settle these matters. Since the present calculation makes no provisions for projection and for cluster initialization it can not be expected to yield reliable predictions for the only kind of parity mixing observed so far, and so that option was dropped altogether. Thus the density matrix occurring in Eq. (2.6) breaks up into 4 sets with pairs of labels (p^+p^+) , (p^-p^-) , (n^+n^+) , and (n^-n^-) , which are conveniently labeled as $\rho_p^{(\pm)}$ and $\rho_n^{(\pm)}$.

Although complete breakdown of rotational invariance was allowed during the iterations, the initial density matrix was always required to transform as some representation of the IV group, under rotations by π radians about any one of the

coordinate axes x , y , or z . Following Bar-Touv and Kelson [45], it can be shown that this suffices to insure that we are in the principal axis system, namely, the one where the expectation value of the mass quadrupole tensor $\sum_{n=1}^A r_i^{(n)} r_j^{(n)}$, $i, j = 1, 2, 3$, is diagonal. This imposes a restriction in the sum over α of Eq. (2.8), in that the values of $m_\alpha - \frac{1}{2}$, for a given l , must be all even or all odd.

The time reversal properties are best described if we adopt the convention [35]

$$T | \phi_\alpha \rangle = s_\alpha | \phi_{\bar{\alpha}} \rangle, \quad (2.27)$$

so that an additional factor of i^L appears [32] in the definition of Y_L^m . Equation (2.27) implies that the two sets defined above are transformed into one another under T . The HF solutions are said to be T symmetric if all HF orbits appear in degenerate pairs whose wavefunctions are mutual T -conjugates, otherwise they will be called T violating. In the T symmetric case only one of the above sets needs be considered [8] and the density matrix can be taken as real and symmetric. This situation can hold only if we have an even number of neutrons and protons. For odd nuclei, both sets of orbital must be computed separately and the density matrix can, in general, be complex hermitian. Our calculation does allow for T violation as defined above and can therefore treat odd and odd-odd nuclei. Another advantage of this method is to facilitate cranking calculations using, say, the 21 generators of the symplectic $Sp(3, 3)$ group [46, 47]. The results of the cranking are outside the scope of this work and will be reported elsewhere.

Since the variational wavefunction obtained in the HF method is a SD, only the antisymmetrisation correlations required by the Pauli principle are included, so that the expectation value of any operator can be expressed [1] in terms of the expectation value of the sp density matrix Eq. (2.11). The nonlocal sp density distribution in coordinate space is

$$\rho(\mathbf{x}, \mathbf{x}') = \sum_{\alpha\beta} \phi_\beta(\mathbf{x}) \rho_{\beta\alpha} \phi_\alpha^*(\mathbf{x}'), \quad (2.28)$$

where $\phi_\beta(\mathbf{x}')$ is the sp wavefunction in the expansion basis. The diagonal part of Eq. (2.28), $\rho(\mathbf{x}) = \rho(\mathbf{x}, \mathbf{x})$, is the usual density function and some results for its values will be give in Section 3.

As pointed out in the Introduction, the symmetries of H which were broken in the HF approximation were not restored later on by the method of projection. This should not affect greatly the bulk properties of the HF ground states but does restrict us, in most cases, to such states only.

H. The Initial Trial Wavefunction

The HF variational equations, like most variational methods, do not necessarily converge to the absolute energy minimum, unless the initial wavefunction is

similar enough to the one which gives that absolute minimum. Thus, considerable prior knowledge of the nuclear properties is required before the further refinement of a self-consistent HF variation can be applied.

We have obtained the initial wavefunctions by using the computer code ELMOS [19], which calculates the *sp* wavefunctions in a ellipsoidal Nilsson [20] type modified oscillator potential and computes the total energy sum for the system of *N* neutrons and *Z* protons *vs.* the β , γ variables of the quadrupole deformation plane. The spin-orbit and l^2 parameters used are those reported in previous work [48]. No Coulomb energies were included in this preliminary construction of the energy surface but major shell mixing in the wavefunction was taken into account. Although it has been contended that the total energy surface of light nuclei [50] is poorly described by the Nilsson model, it is usually conceded that the model surface has an absolute minimum at the correct values of β and γ and that the wavefunction at this point is a reasonable approximation for our purpose.

Still, there are nuclei, mainly those with $24 \leq A \leq 36$, for which several minima of comparable energy are observed. In those cases, HF iterations were performed starting from each minimum and the case resulting in lowest HF result was identified and is reported here (Section 3.A).

3. RESULTS AND SYSTEMATICS

Introduction

Some results of the HF calculations for 57 nuclei from ^4He to ^{41}Sc are presented in Table II. These nuclei are those for which $N - Z = 0, \pm 1$, and suffice to illustrate the systematics in this region of the periodic table. All entries are ground state configurations except the two labeled $^{12}\text{C}^*$ and $^{16}\text{O}^*$ which are excited intrinsic states. The entries of each column are as follows: $\hbar\omega$ is the oscillation frequency of the basis wavefunctions, β_0 and γ_0 are input data for the initialization and are the approximate values of the deformation parameters where a minimum in the Nilsson total energy is observed. The Nilsson potential is the same for both protons and neutrons so that only one set of values are required. Next listed are the total HF binding energy W , and the total and direct Coulomb energy, W_c and W_{cd} , respectively. The following six entries give the *sp* energies of lowest occupied state ϵ_1 ($\sim 0s_{1/2}$ state), that of the highest occupied state ϵ_f (the Fermi energy) and that of the first unoccupied state ϵ_{f+1} , for the neutrons and protons, respectively. The next 9 entries describe the diagonal *sp* mass quadrupole properties of the proton, neutron and total ($p + n$) HF density distributions. The method for extracting the rms radius, β and γ from the mass quadrupole components is given in Ref. [49]. The next two entries list the rms radii, with respect to the total c.m., of the proton and total density distributions, respectively. These last two

numbers are independent of the details of the wavefunction of the c.m. of the system. Next is the proton intrinsic quadrupole moment in barns. Finally, the isospin impurity for the $N = Z$ nucleus is given.

Most of these entries are discussed separately in the following subsections and compared with experiment wherever possible or with the predictions of other models. The emphasis has been put on the systematics of the calculated results, and individual cases are discussed only when anomalies are observed, thus graphical presentation of the results as a function of atomic number is used repeatedly. Simple formulas, as functions of A and/or Z , are deduced from the HF results and presented, whenever deemed interesting; they may be used to extrapolate to mass regions not discussed here.

Subsections A dispatches matters related to the basis dependence of the calculation while the next five subsections concern themselves with quantities immediately related to experiment. Having checked that we indeed seem to account adequately for the better-known properties of the nuclei in this mass region, the last three subsections exploit the detailing power of the model in order to make predictions about isospin-related quantities whose experimental observation is more difficult to make directly.

A. Dependence on the Basis Oscillator Frequency

The HF results will not depend on the oscillator frequency $\hbar\omega$ of the basis states if the number of those states included in the expansion Eq. (2.8), is made sufficiently large. However we learn from Eq. (2.10) that the number of operations required for one iteration grows as the fourth power of the basis size. Thus one must truncate the basis to the smallest size which will give reasonable convergence of the results, at the expense of introducing an appreciable dependence on $\hbar\omega$. One then treats $\hbar\omega$ as an additional variational parameter to be selected so that maximum binding is obtained.

Since the initial trial wavefunction is a Nilsson type SD one must expect that $\hbar\omega$ should be chosen to make it as good a wavefunction as possible. It is well known, however, that the value $\hbar\omega \approx 41 \text{ MeV}/A^{1/3}$ then represents an adequate choice for nuclei near the β -stability line. This yields the first order estimates of $\hbar\omega$ for ${}^4\text{He}$, ${}^{16}\text{O}$, and ${}^{40}\text{Ca}$, of 26, 16, and 12 MeV, respectively. For practical reasons the matrix elements of the potential were calculated for the values $\hbar\omega = 8.0, 10.5, 13.5, 15.0, 17.5, 20.0, 25.0$, and 30 MeV, in order to bracket the above first-order estimates. These values were then used to compute the binding energy of selected nuclei in the range of interest. This was first done in a smaller basis consisting of the first three oscillator major shells (Fig. 2) and next in the full working basis (Fig. 3) of five major shells described in Table I, in order to exhibit the effects of extreme basis truncation. Figure 2 shows that the dependence of W on $\hbar\omega$ increases with the mass. The curve labeled ${}^{12}\text{C}^*$ show a break which indicates

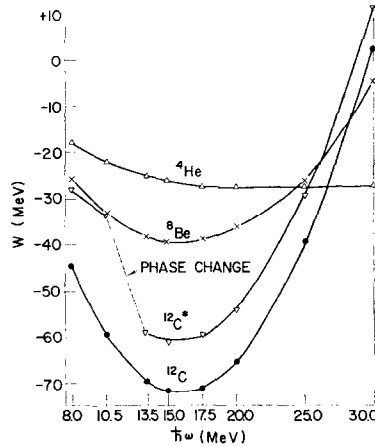


FIG. 2. Binding energy (W) vs. $\hbar\omega$ curves for ${}^4\text{He}$, ${}^8\text{Be}$, ${}^{12}\text{C}$ and ${}^{12}\text{C}^*$ calculated in the three major shell basis.

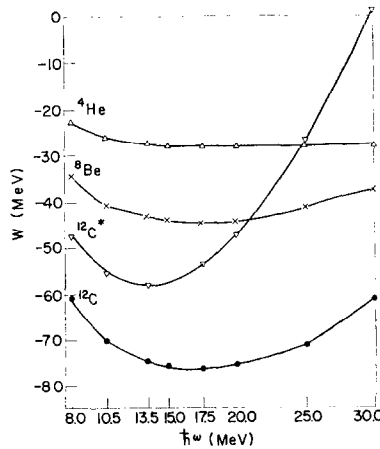


FIG. 3. Binding energy vs. $\hbar\omega$ curves for ${}^4\text{He}$, ${}^8\text{Be}$, ${}^{12}\text{C}$ and ${}^{12}\text{C}^*$ calculated in the five major shell basis.

that the initial configuration $(n_1, n_2, n_3) = (0, 0, 0)^4 (0, 0, 1)^4 (0, 0, 2)^4$, of three alpha particles in a line is not stable at all values of $\hbar\omega$, in such a small basis. Figure 3 shows a marked decrease of the dependence on $\hbar\omega$ and a slight shift of the minimum towards higher $\hbar\omega$, as well as an energy gain at the minimum. As expected, the energy gain is larger for the more strongly deformed nuclei, presumably because they induce stronger major shell mixing. The in-line configuration of ${}^{12}\text{C}^*$ is now stable; it occurs here at ~ 19 MeV excitation in ${}^{12}\text{C}$ but it is generally associated [50] with the 7.65 MeV excited state of ${}^{12}\text{C}$. We will return to this matter later on. Figure 4 shows the $\hbar\omega$ dependence of the binding energy per

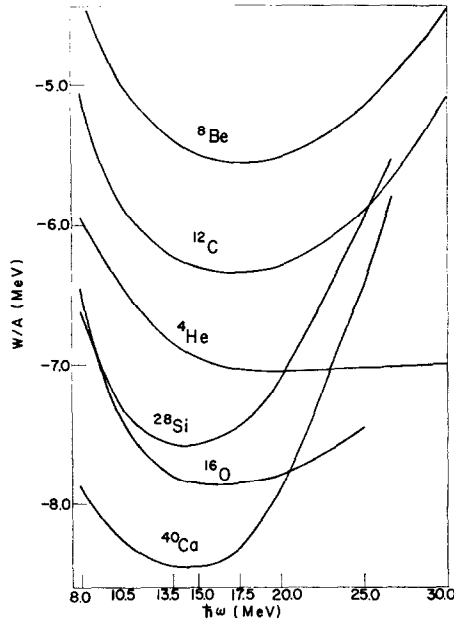


FIG. 4. Binding energy per nucleon vs. $\hbar\omega$ curves for some nuclei calculated in the five major shell basis.

nucleon for the ground state of several even-even nuclei from ${}^4\text{He}$ to ${}^{40}\text{Ca}$. Again we notice that the dependence increases with the mass and is stronger for the more deformed nuclei such as ${}^8\text{Be}$, ${}^{12}\text{C}$, and ${}^{28}\text{Si}$. As a result of this study, we have assigned optimum values of $\hbar\omega$ to the various mass regions in the manner given in Table III. For those series of isotopes of a given nucleus in Table II which fall on the boundaries of Table III, the results obtained from using the larger and smaller values of $\hbar\omega$ are both presented in Table II.

TABLE III
Optimum Values for $\hbar\omega$

A	4 – 5	5 – 13	13 – 29	29 – 40
$\hbar\omega(\text{MeV})$	20.0	17.5	15.0	13.5

An additional test of the basis is displayed in Fig. 5 where the rms radii of some nuclei are plotted as functions of the oscillator parameters $b = (\hbar/m\omega)^{1/2}$. In the extreme truncation limit where the wavefunction is a pure oscillator state, the

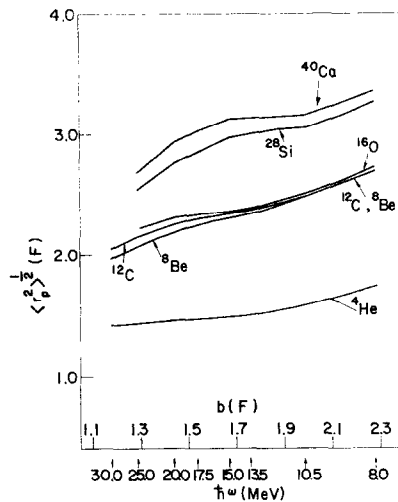


FIG. 5. Calculated rms radii of the proton distributions for some nuclei vs. the oscillator size parameter $b = (\hbar/M\omega)^{1/2}$.

radius would be proportional to b , but in a large enough basis it would be independent of b . Although the dependence on b is evident, it is much weaker than a linear one; this is especially so in the neighborhood of the optimal $\hbar\omega$, in each case considered. We conclude from these tests that although some improvement would undoubtedly result from using a still larger basis, the present one is adequate to account quantitatively for the systematic intrinsic properties of the light nuclei.

B. Ground-State Binding Energies

The calculated HF binding energies per nucleon $-W/A$ (light lines) are shown in Fig. 6, and compared with the experimental data [51] (heavy lines). The well-known systematics of the empirical data has been rather well reproduced. However, the ratio $W_{\text{HF}}/W_{\text{exp}}$ shows a systematic underbinding as A departs from the magic numbers 4, 16, and 40. Inspection of Table II shows some measure of correlation between the amount of underbinding and the equilibrium deformation parameter β . It is known that the binding energy of a state projected from a strongly deformed one will increase over that of the intrinsic state alone, although the typical energy gains reported so far [52] have been in the range 2–10 MeV whereas the discrepancy in W here is sometimes as large as 36 MeV. It is probable that some of the missing energy for the deformed nuclei could be recovered by going to a still larger basis, since it was pointed out in Subsection A that deformed states do require a larger spherical basis for their proper expansion. The relative importance of angular

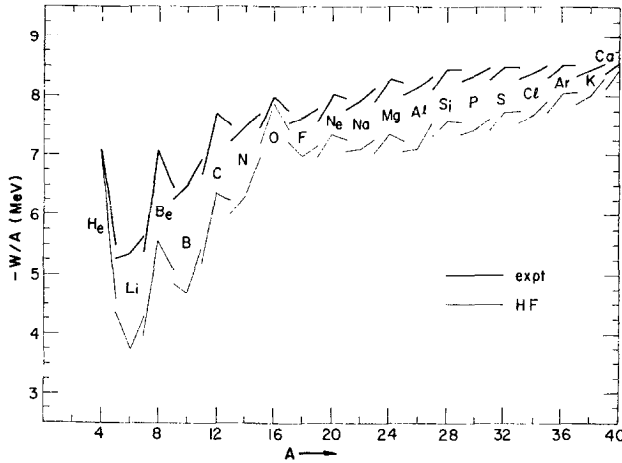


FIG. 6. Systematics of the calculated (thin lines) and experimental [51] (heavy lines) binding energy per nucleon.

momentum projection and basis truncation will be the subject of a future investigation.

C. Separation and Fermi Energies

The single-proton $S_p(N, Z)$ and single-neutron $S_n(N, Z)$ separation energies are defined as

$$S_p(N, Z) = -[W(N, Z) - W(N, Z - 1)], \quad (3.1a)$$

$$S_n(N, Z) = -[W(N, Z) - W(N - 1, Z)]. \quad (3.1b)$$

These exact definitions, which use finite differences, may be approximated by using the derivatives of W as pointed out in Section 2.E; Eq. (II.26) then supplies the approximations $S_p \approx -\epsilon_f^p$, $S_n \approx -\epsilon_f^n$, in terms of the proton and neutron Fermi energies, the energies of the last occupied states. The exact relation between ϵ_f and W can be obtained in the HF approximation by using Eq. (2.12) to write

$$W(A) = \sum_{i \neq f} T_{ii} + \frac{1}{2} \sum_{i, j \neq f} v_{ijij} + T_{ff} + \sum_i v_{ifif}, \quad (3.2)$$

where the antisymmetry properties of v_{ijkl} has been used and imply $v_{ffff} \equiv 0$. The first two sums only involve $A - 1$ nucleons and must therefore represent the energy $W^*(A - 1)$ of some excited state of the $A - 1$ nucleon system, *provided H is independent of A* , while the remainder is just ϵ_f , according to Eq. (2.7); thus we have

$$W(A) = W^*(A - 1) + \epsilon_f. \quad (3.3)$$

Should the HF orbits of the $A - 1$ system coincide with those of the A system, we would have $W^*(A - 1) = W(A - 1)$, otherwise we put

$$W^*(A - 1) = W(A - 1) + \Delta(A - 1), \quad \Delta \geq 0, \quad (3.4)$$

where Δ , the HF rearrangement energy, must be nonnegative if both HF calculations for A and $A - 1$ are absolute minima. Collecting the above results we obtain the relations

$$S_p(N, Z) = -\epsilon_f^p(N, Z) - \Delta_p(N, Z - 1), \quad (3.5a)$$

$$S_n(N, Z) = -\epsilon_f^n(N, Z) - \Delta_n(N - 1, Z). \quad (3.5b)$$

For very heavy nuclei the structure of the occupied orbits will not be changed appreciably by adding one nucleon, because this then represents a small perturbation on the average field, so that Δ will be negligible. We note that if we were to compute S from projected wavefunctions instead of HF Slater determinants, it could no longer be separated exactly into a Fermi energy and a rearrangement energy as in Eqs. (3.5) since, as discussed in the Introduction and illustrated in Fig. 1, the Fermi level could no longer be singled out uniquely.

The calculated values of $-\epsilon_f^n$ are compared with the experimental neutron separation energies [51] in Fig. 7(a), for $N = Z$ nuclei, in the case of even A , and

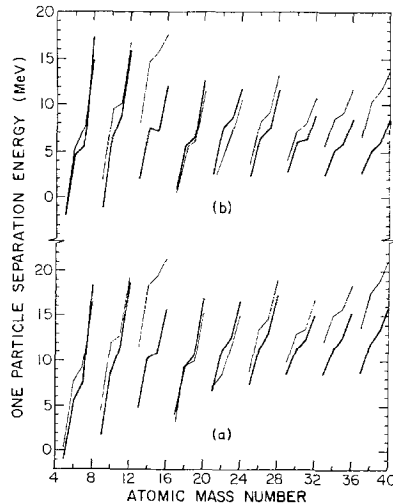


FIG. 7. (a) Systematics of the computed values of $-\epsilon_f^n$ (light lines) and the empirical one-neutron separation energies (heavy lines). $N = Z$, when A is even; otherwise $N = Z + 1$. (b) is the proton counterpart of (a).

for $N = Z + 1$ nuclei otherwise. The proton counterpart of this display is shown in Fig. 7(b). The two graphs are very similar and will be discussed together.

The systematics of the empirical separation energies are generally well reproduced by $-\epsilon_f$, the largest deviations being near the closed shells; this effect is related to

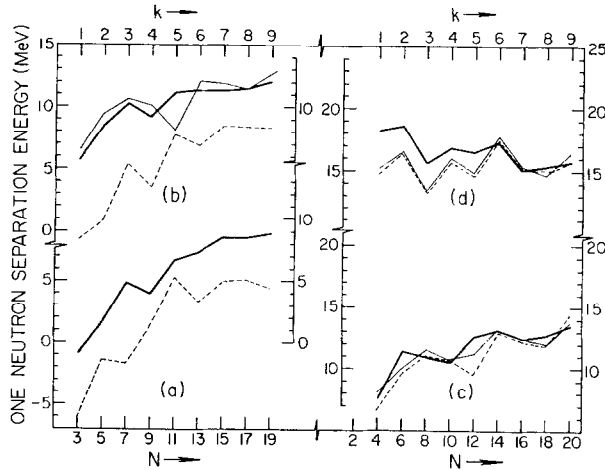


FIG. 8. Comparison of the empirical one-neutron separation energies (heavy lines) and the calculated values of S_n (dashed lines) and $-\epsilon_f^n$ (light lines) for (a) $A = 4k + 1$, $N = Z + 1$, (b) $A = 4k + 2$, $N = Z$, (c) $A = 4k + 3$, $N = Z + 1$, and (d) $A = 4k + 4$, $N = Z$ nuclei. The computed values are shifted such that in (a) $-\epsilon_f^n$ coincides with the corresponding experimental separation energy for each value of k .

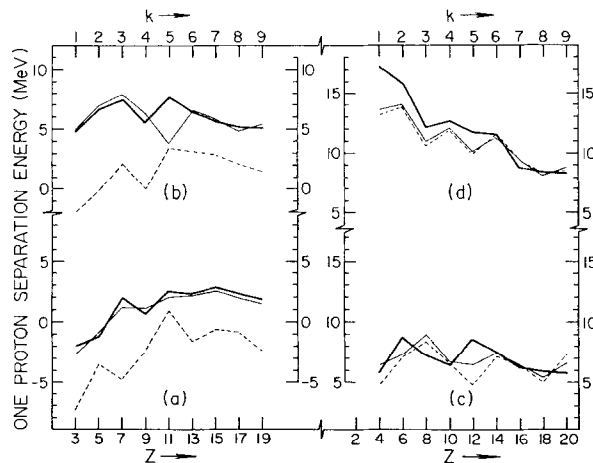


FIG. 9. Proton counterpart of Fig. 8. The theoretical values of $-\epsilon_f^p$ and S_p are shifted by the same amount as the corresponding $-\epsilon_f^n$ is shifted in Fig. 9(a).

the missing rotational correlation energy which changes most rapidly in these regions, as discussed in subsection A.

More detailed comparisons of the calculated values of S and $-\epsilon_f$ with the experimental separation energies are shown in Figs. 8 and 9, for neutrons and protons, respectively. In these figures, the nuclei are classified into four groups, where in each group $A = 4k + i$, k integer and $i = 1, 2, 3$ or 4 . In order to remove the discrepancy due to the missing rotational correlation energy so that discrepancies arising from other sources may be detected, all calculated values of S and $-\epsilon_f$ have been shifted such that the value of $-\epsilon_f^n$ agrees with the experimental datum for each $A = 4k + 1, N = Z + 1$ nucleus. It is seen that the overall agreement between the shifted values of $-\epsilon_f$ and the empirical data is good. In particular, most of the pairing correlation energy seems to be accounted for. One notes that while for the $4k + 3$ and $4k + 4$ nuclei the corresponding values of S and $-\epsilon_f$ are very nearly equal, for the $4k + 1$ and $4k + 2$ nuclei they are characteristically separated by $4 \sim 7$ MeV. Since the states with an odd number of neutrons and/or protons are T violating whereas the even-even ones are not, an additional correlation energy should be recovered by the projection method, much in the same way as the rotational correlation energy. In those cases we may suppose that an energy $\delta_n = |\delta|$ for the odd neutron and $\delta_p \cong \delta_n$ for the odd proton would be gained so that the $4k + 3$ and $4k + 4$ nuclei, in Figs. 8 and 9, would see their separation energy decreased by $|\delta|$ while the $4k + 1$ and $4k + 2$ ones would suffer an increase by the same amount, thus reducing the disagreement between the systematics of the difference $(-\epsilon_f) - S$ for $4k + 1$ and $4k + 2$ nuclei and for $4k + 3$ and $4k + 4$ nuclei. Closer inspection of Figs. 8 and 9 shows that for $A = 21$ and 22 the differences $-\epsilon_f - S$ are exceptionally small. Conversely we see, from Table IV,

TABLE IV
Overlaps of the Wavefunctions of the Last Bound Neutron States and Their
(Unoccupied) " T -conjugate" in Odd-Odd Nuclei

${}^6\text{Li}$	${}^{10}\text{B}$	${}^{14}\text{N}$	${}^{18}\text{F}$	${}^{22}\text{Na}$
0.99564	0.99121	0.98355	0.97841	0.99934
${}^{26}\text{Al}$	${}^{30}\text{P}$	${}^{34}\text{Cl}$	${}^{38}\text{K}$	
0.98657	0.99453	0.99558	0.97579	

that for $A = 22$ the last neutron orbit has the largest overlap with its corresponding unoccupied time-reversed orbit of all the odd-odd nuclei considered. It is interesting to note that after correcting S by $|\delta|$, as explained above, all the rearrangement

energies are positive and would be of order 2–3.5 MeV in most cases. More precise estimates of this experimentally unobservable model quantity must await a full treatment of projection from T -violating HF solutions.

We conclude this section by observing that although the gross features of Fig. 7 can already be observed in the ellipsoidal Nilsson model [21], it is gratifying to find that considerable improvement has been obtained by using the HF results, where no empirical information other than the properties of nuclear matter and those of the two-nucleon system have been used explicitly.

D. Density Distribution and Alpha Particle Clustering

High energy electron scattering [53–56] has proved to be a powerful tool in the study of the form factor of the charge density distribution of nuclei, and has yielded a considerable amount of information on its properties such as its rms radius, surface thickness and central value. The density distributions $\rho(r)$ obtained here are spherically symmetric for the magic nuclei ^4He , ^{16}O and ^{40}Ca and are thus functions of $|\mathbf{r}| = r$ only. The Fig. 10 shows a graph of the total density *vs.* r for these 3

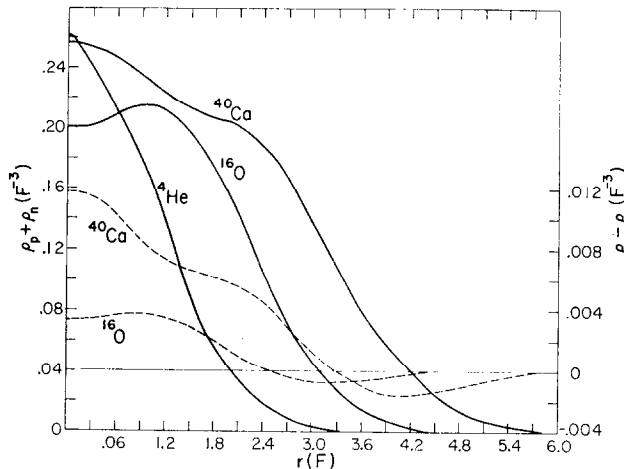


FIG. 10. Radial density distributions for ^4He , ^{16}O , and ^{40}Ca . The solid lines are $\rho_p(r) + \rho_n(r)$, and the dashed lines, $\rho_p(r) - \rho_n(r)$.

nuclei. In addition the difference between the proton and neutron density for ^{16}O and ^{40}Ca is also given there, so that the proton density alone may be obtained and folded with the proton charge density to obtain the total charge density. The central densities shown here are larger than the value 0.17 nucleon per cubic Fermi currently accepted for nuclear matter [57], and also larger than those predicted by using density-dependent two-body interactions [11]. Each of these nuclei will now be examined separately.

For ${}^4\text{He}$, the empirical density distribution extracted from e -scattering [58] is quite high at the center even after correction for the repulsive, short-range, two-body correlations; this plus the fact that our predicted value for the rms proton radius (Fig. 26) is in good agreement with experiment suggest that the central peaking in ${}^4\text{He}$ may be a real effect, consistent with the tightly bound nature of that nucleus. Corresponding to the high central densities of ${}^{16}\text{O}$ and ${}^{40}\text{Ca}$, we note from Fig. 26 that the predicted values of their rms proton radii are too small by about 0.25 fm. A possible explanation of this effect may be that we are not able to exclude, on the basis of simple rotational-vibrational model arguments, the possibility that a sizeable zero-point vibration needs be included in the description of the ground state of these nuclei; this would increase the rms radius and decrease the central density. In the case of ${}^{16}\text{O}$, the vibration would mainly admix into the ground state the much larger diamond-shaped configuration of Fig. 25, while for ${}^{40}\text{Ca}$ a larger number of configurations would be brought in, in accord with the belief that ${}^{40}\text{Ca}$ is only nominally a closed shell nucleus.

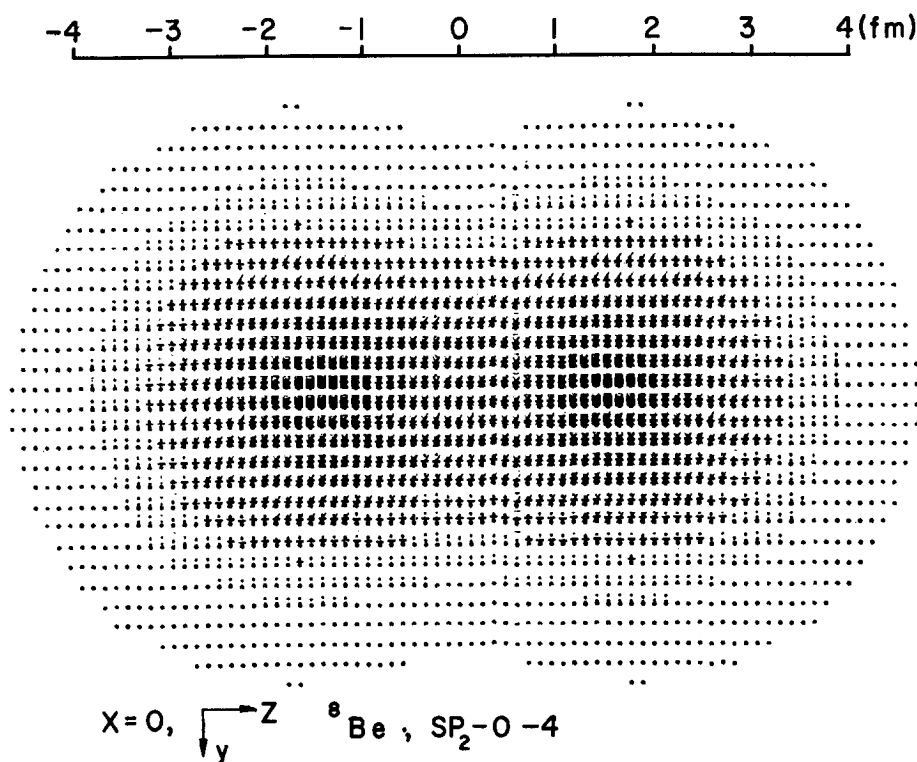


FIG. 11. "Photographic" plot of the total density for ${}^8\text{Be}$ in the $x = 0$ plane. The "blackness" of any area is roughly proportional to the density.

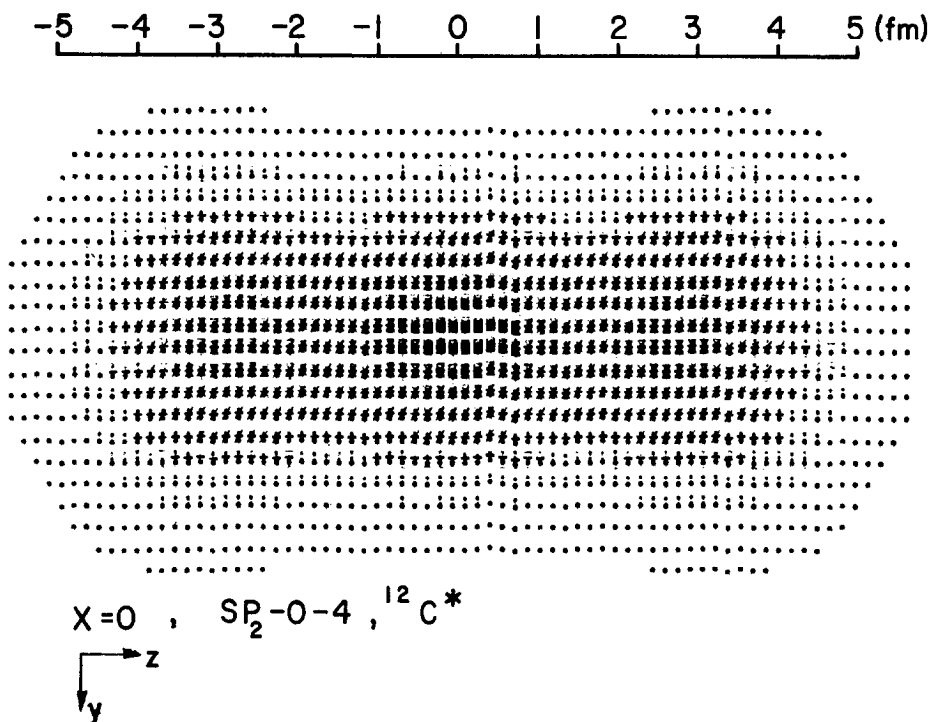


FIG. 12. Same as in Fig. 11, but for $^{12}C^*$.

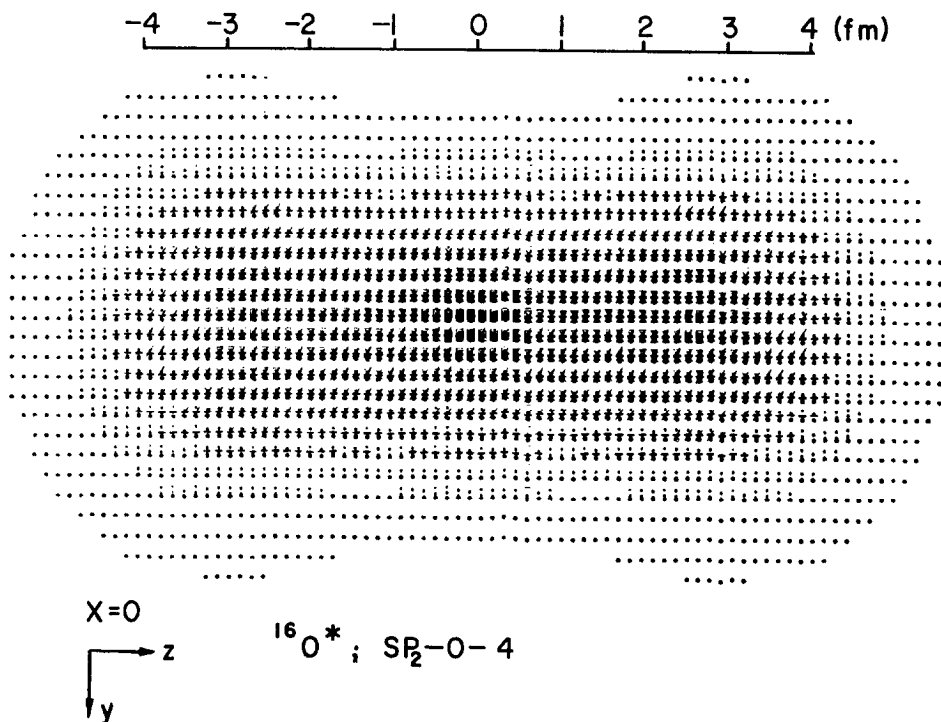


FIG. 13. Same as in Fig. 11, but for $^{16}O^*$ in the $x = 0$ plane.

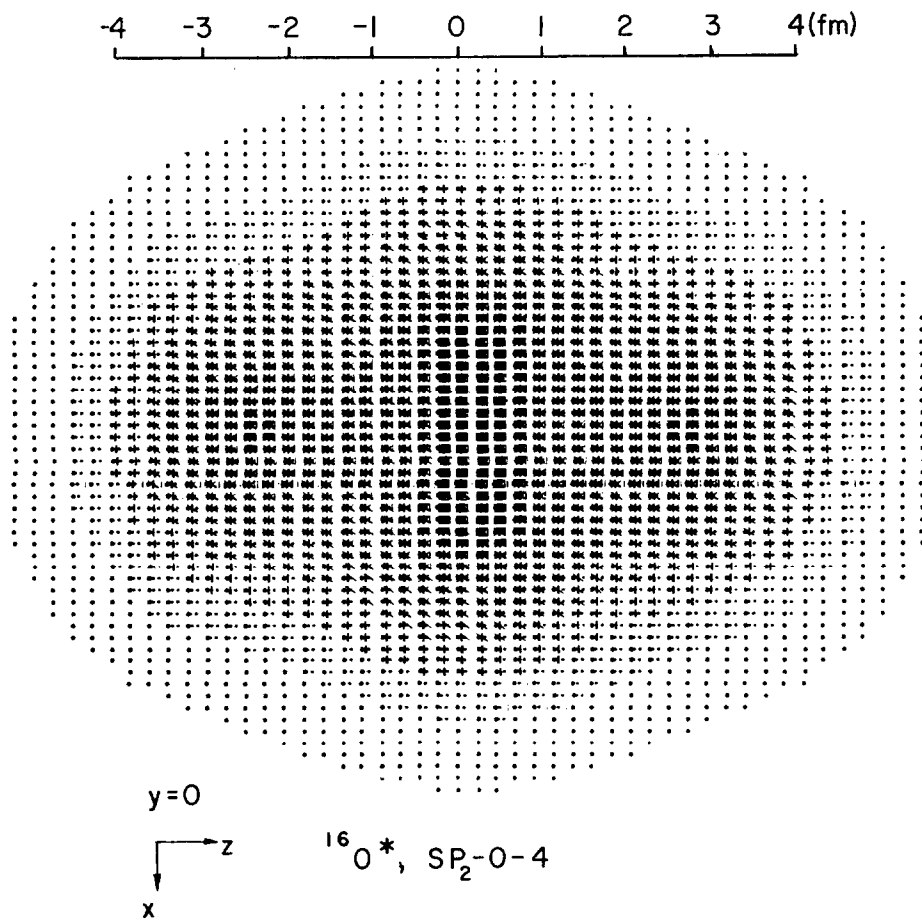


FIG. 14. Same as in Fig. 11, but for $^{16}\text{O}^*$ in the $y = 0$ plane.

The density distribution $\rho(\mathbf{r})$ for several deformed nuclei are shown in Figs. 11–16 as intensities in various planes cut across the nucleus. A cut in the $x = 0$ plane ^8Be is shown in Fig. 11; the two α clusters in near contact are easily recognized since the density half-way between their centers is some 30 % lower than the maximum values at the centers. Although ^8Be is unstable towards fission into two α -particles, it is probable that the Coulomb barrier keeps them together and that the HF calculation is insensitive to the fission process. Fig. 12 shows a cut in the $x = 0$ plane of $^{12}\text{C}^*$, the in-line three- α cluster excited intrinsic state mentioned earlier. Again the two saddle-point densities are about 30 % lower than the peak densities. Our next example of clustered deformed nuclei is illustrated in Figs. 13, 14, 15 where cuts in the $x = 0$, $y = 0$ and $z = 0$ planes of the nonaxial $^{16}\text{O}^*(4p-4h)$ state

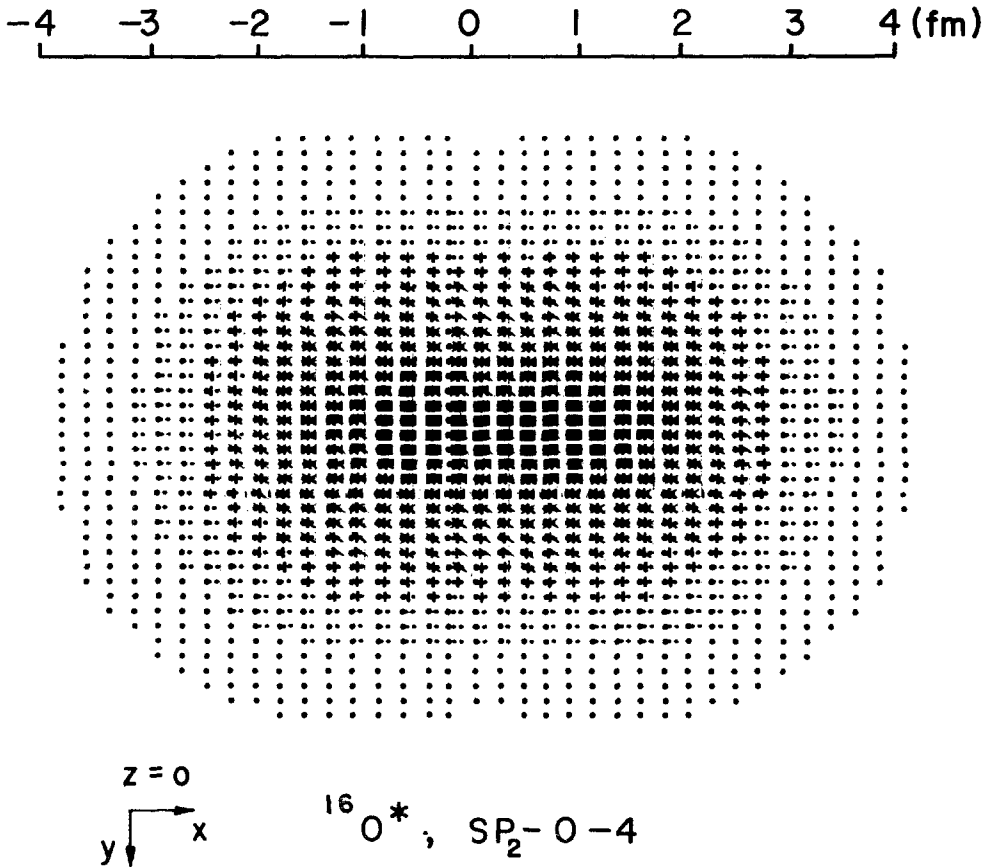


FIG. 15. Same as in Fig. 11, but for $^{16}\text{O}^*$ in the $z = 0$ plane.

[59, 60], have been made. Whereas we find the intrinsic excitation energy of this state to be 33 MeV, the O^+ state projected from it occurs experimentally at 6.06 MeV excitation. The ratio of computed to observed binding energy for $^{16}\text{O}^*$ and $^{12}\text{C}^*$ are thus comparable to those obtained for other strongly deformed nuclei as can be seen in Fig. 6; indeed, there is no reason to expect they would behave any differently under projection than the strongly deformed ground states of other nuclei. Our last example show the density in the $x = 0$ plane of ^{20}Ne . The presence of a sizeable hexadecapole deformation will be noticed and could lead to novel effects in reorientation measurements [61] performed on the ground state rotational band of ^{20}Ne .

The quantitative features found in heavier nuclei are more clearly displayed by plotting equi-density contours. The nucleus ^{24}Mg is studied in Figs. 17–20 and ^{32}S

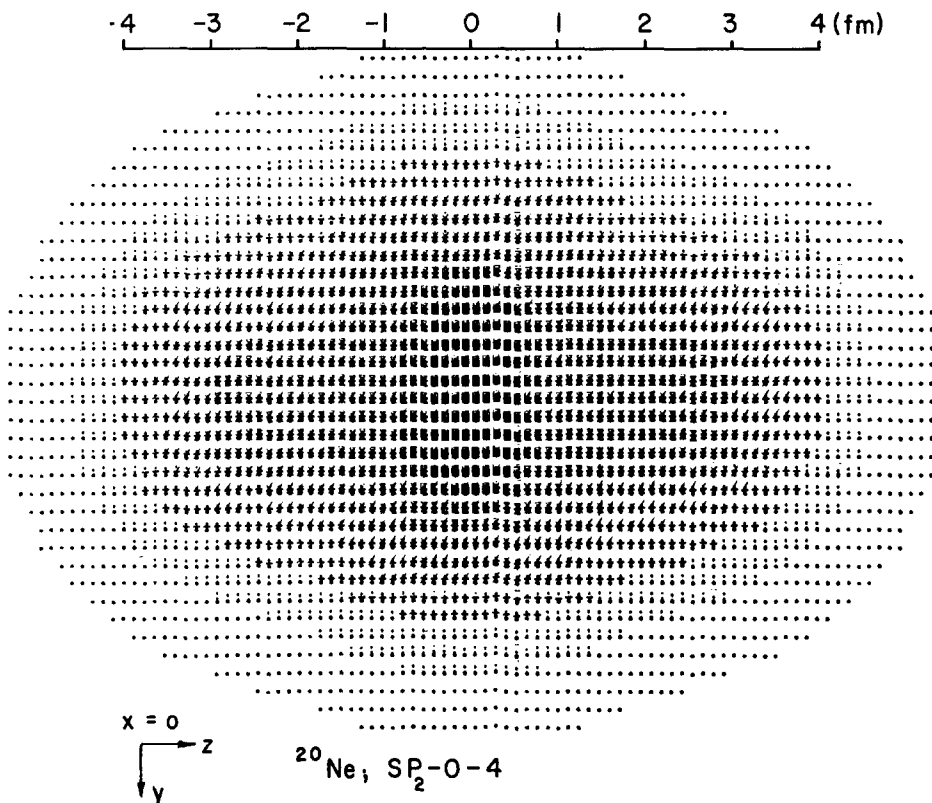


FIG. 16. Same as in Fig. 11, but for ^{20}Ne in the $x = 0$ plane.

in Figs. 21–23. Again cuts are made in some plane parallel to one of the coordinate axes but only one quadrant of the plane is displayed, since the others can be obtained by reflexion, on account of the IV group and parity symmetries discussed earlier. The density concentrations are now less marked and indeed can no longer be associated with α clusters, for $A > 24$. We have compared, in Fig. 24, the densities along a line starting from the center of some clusters, to the radial density of ^4He , as a check of the clustering assumption. Good agreement with the α -particle density is obtained for ^8Be , $^{12}\text{C}^*$, $^{16}\text{O}^*$, whereas the results are beginning to show a marked difference for ^{20}Ne and ^{24}Mg .

We have summarized our results on α clustering in Fig. 26 where six configurations for some light nuclei are illustrated. The parity-violating lattices for ^{12}C and ^{20}Ne are not obtained directly from the HF results but rather are those suggested by Brink *et al.* [16]. The lattice distances shown in Fig. 25 are determined by demanding that they reproduce the rms radius and quadrupole moment

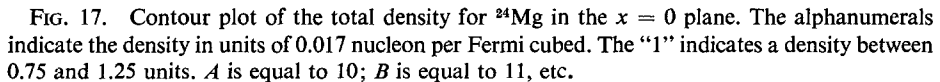


FIG. 18. Same as in Fig. 17, but for ^{24}Mg in the $y = 0$ plane.

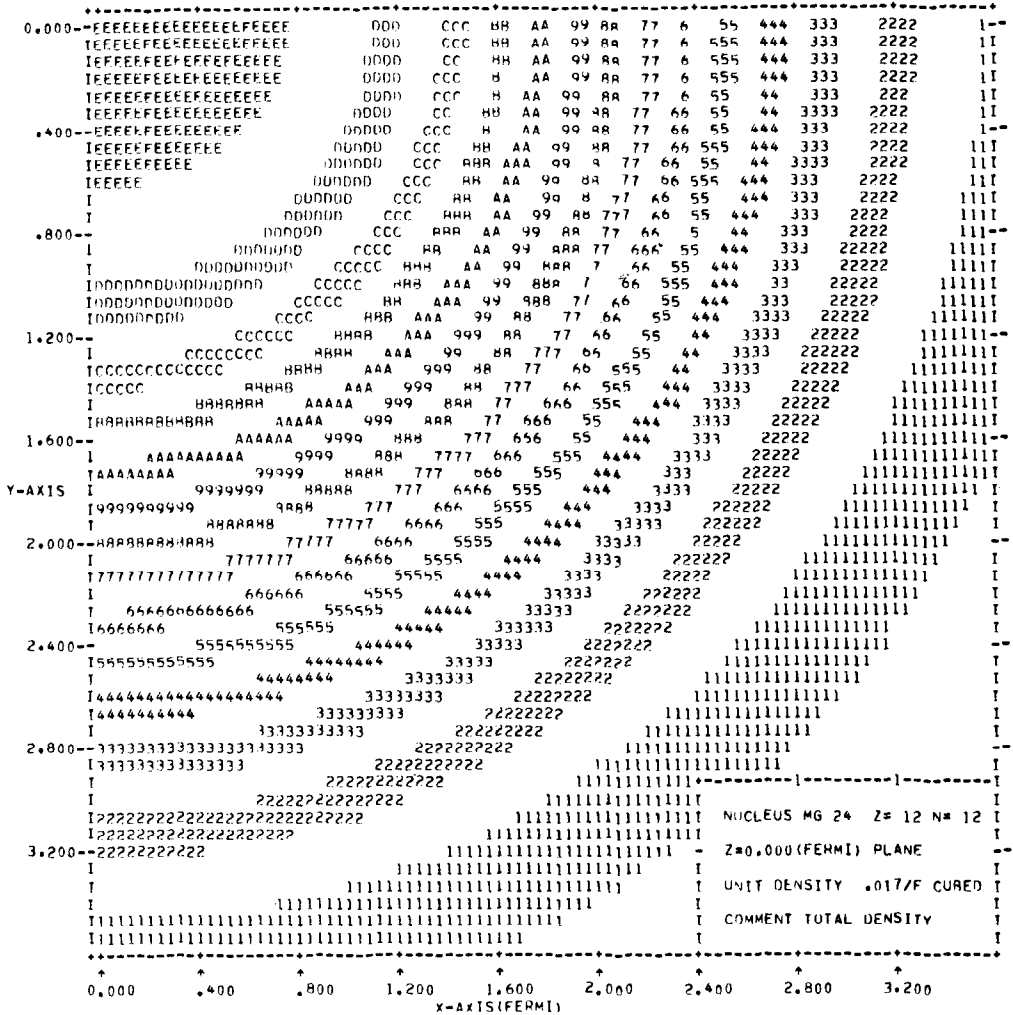


FIG. 19. Same as in Fig. 17, but for ^{24}Mg in the $z = 0$ plane.

[illegible]

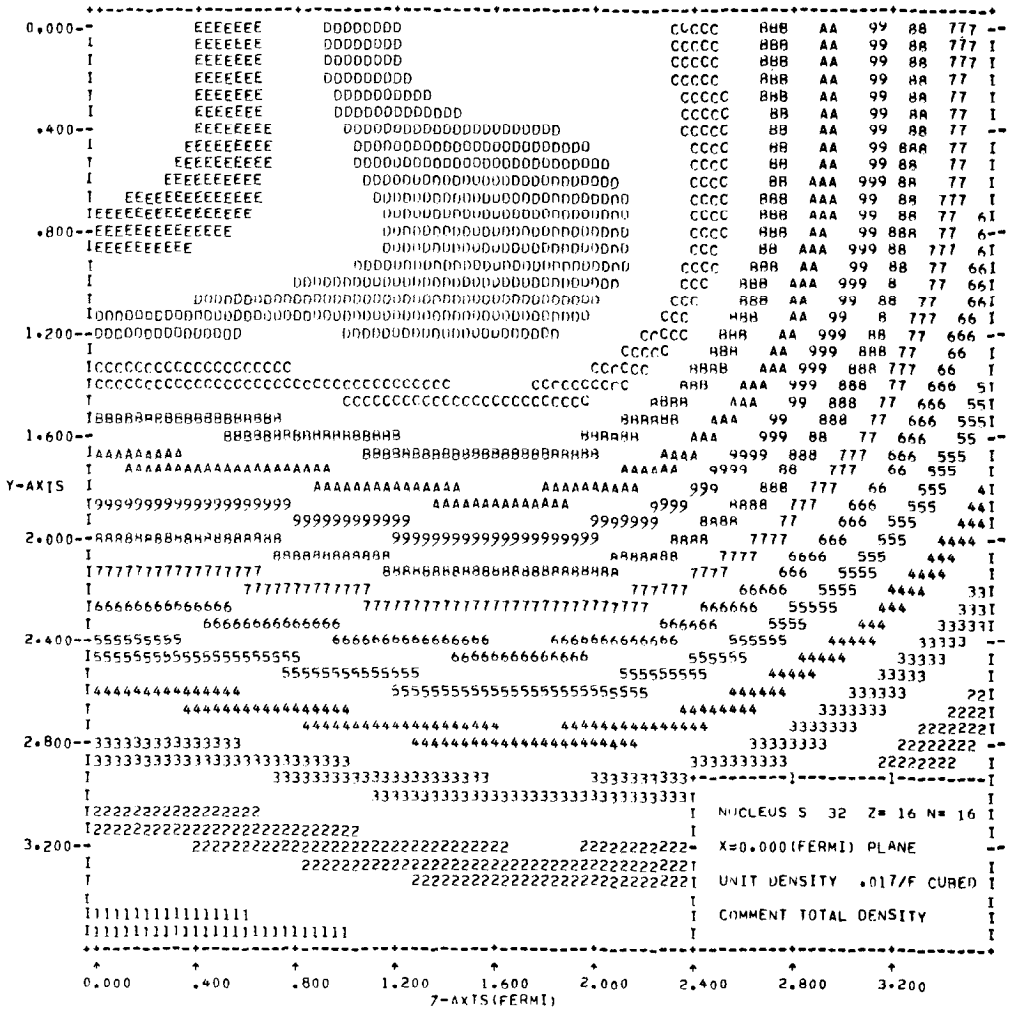
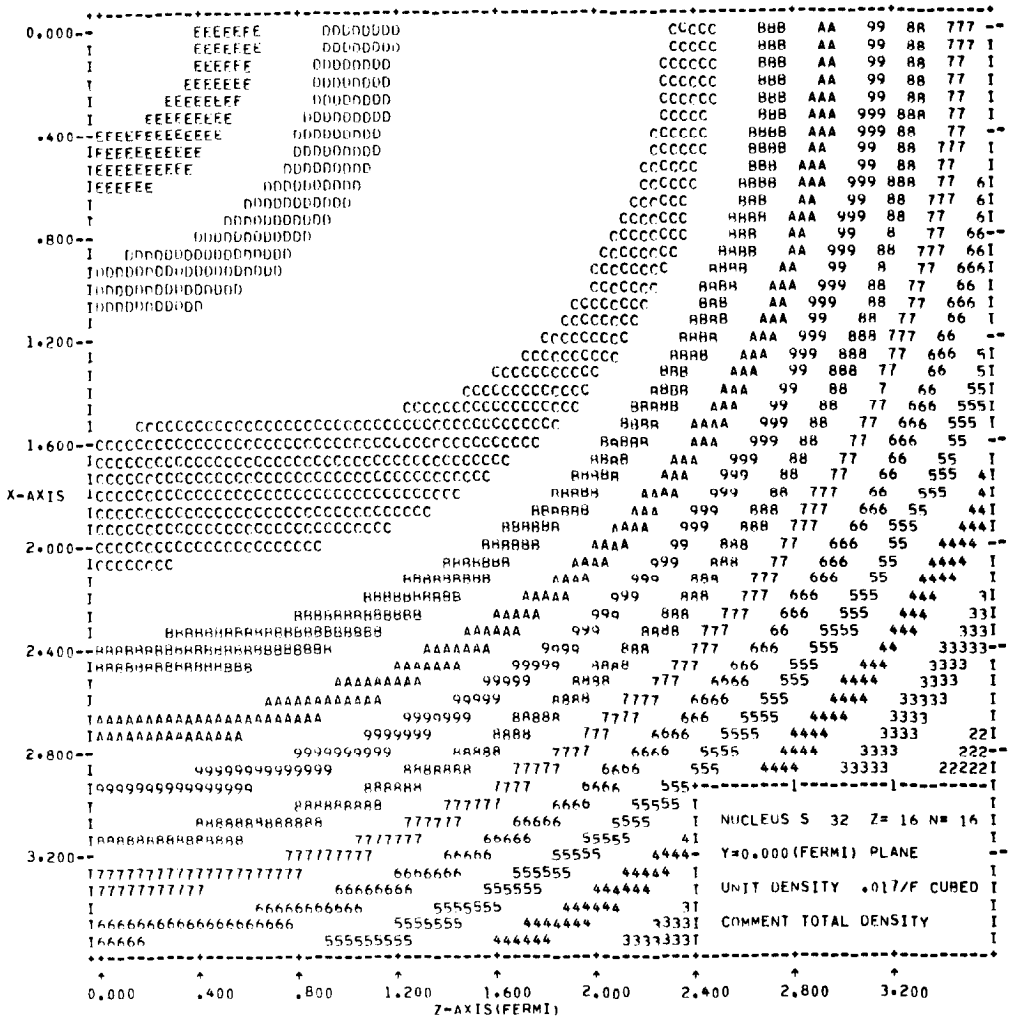


FIG. 21. Same as in Fig. 17, but for ^{32}S in the $x = 0$ plane.

FIG. 22. Same as in Fig. 17, but for ^{32}S in the $y = 0$ plane.

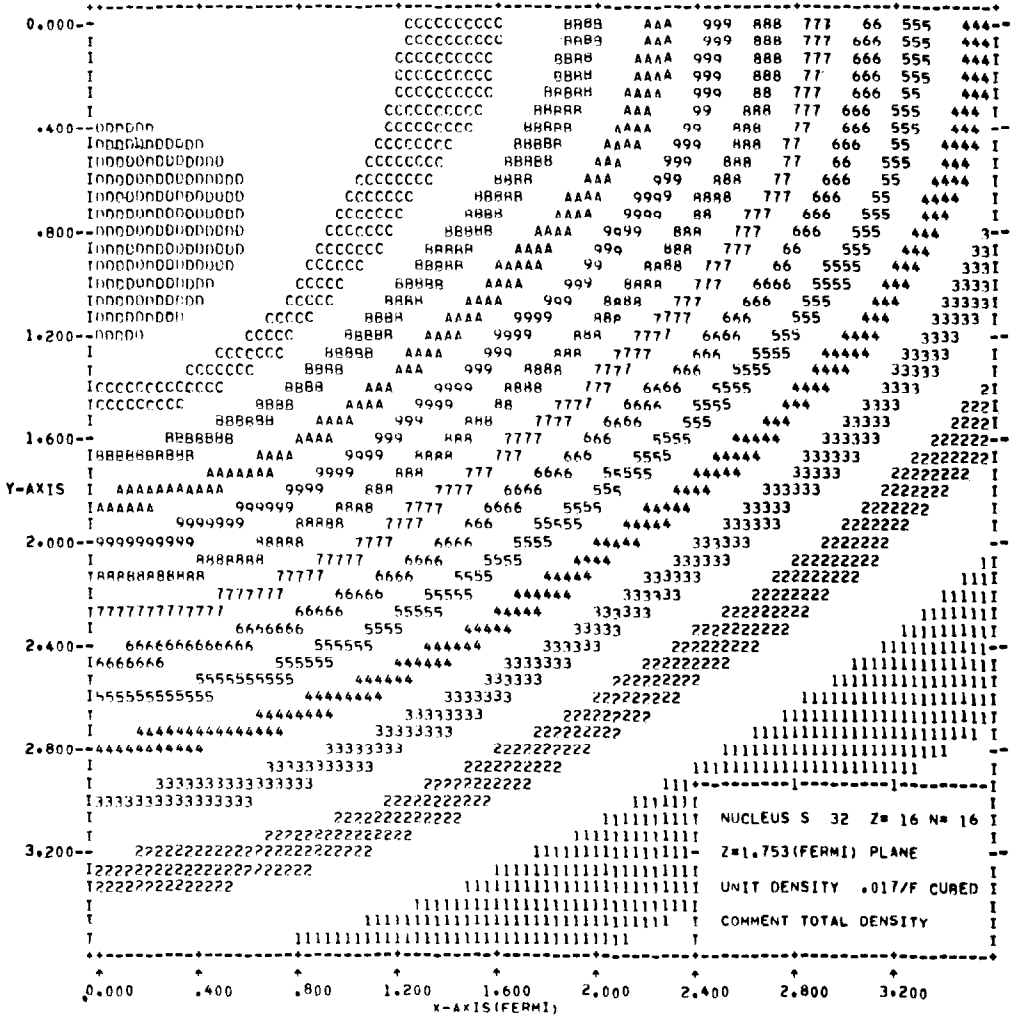


FIG. 23. Same as in Fig. 17, but for ^{32}S in the $z = 1.753$ F plane.

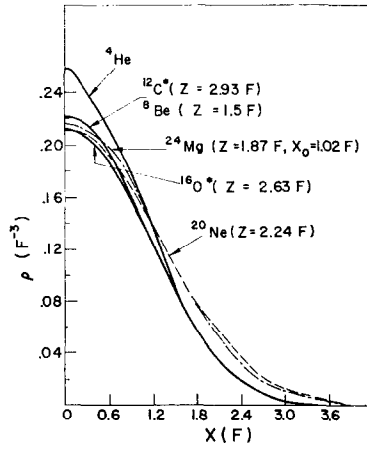


FIG. 24. Total densities of ${}^4\text{He}$ and of some “ α -particle cluster” in some even-even nuclei. The abscissa X is the intersection of the planes $y = 0$ and $z = \text{constant}$ shown in the bracket following each nucleic name ($z = 0$ for ${}^4\text{He}$). The origin of X is $x = 0$, except for ${}^{24}\text{Mg}$, in which case it is $x = 1.02$ F.

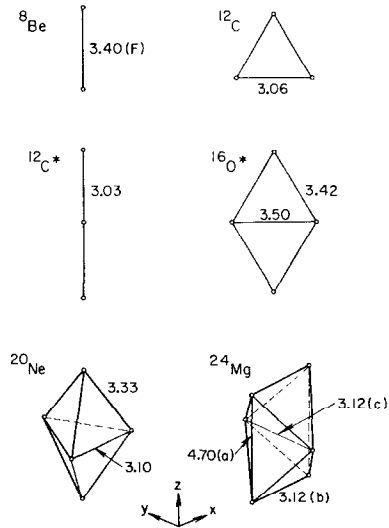


FIG. 25. Probable α -particle structures for some light nuclei.

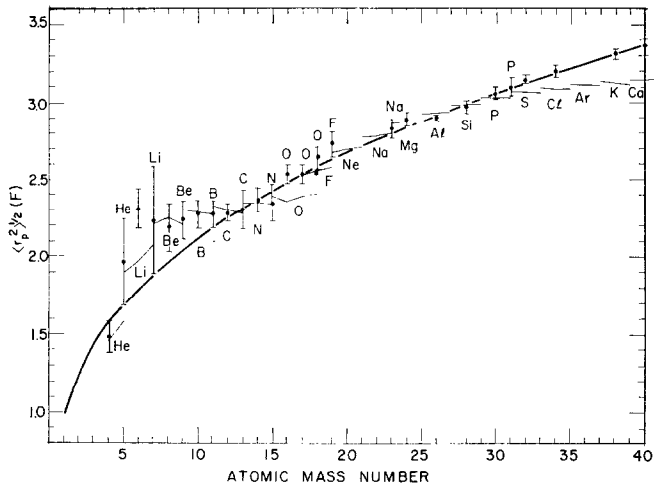


FIG. 26. Calculated and experimental rms radii for the proton density distributions. The experimental data are taken from Refs. [63, 65, 66].

obtained from the HF method for each nucleus. For ^{24}Mg , this criterion uniquely determines the distance a (see Fig. 26), but only requires that $2b^2 + c^2 = 7.4 F^2$. In this case we set $b = c$ as suggested by the density plots, Figs. 18–21. We notice in Fig. 25 that the two-alpha bond is characterized by an almost uniform lattice distance of $3 \sim 3.5F$. Furthermore, the structure of ^{20}Ne is very close to that formed by two tetrahedrons sharing a common base, and ^{24}Mg is formed by two tetrahedrons sharing a common edge. This suggests a predominance of the tetrahedral structure for four interacting alpha particles [59].

E. rms Charge Radii

The Coulomb interaction was recognized early as an extremely useful tool for probing the charge distribution of nuclei. The systematic use of Coulomb energy differences [62] has developed [63] to the point of making extensive predictions concerning the nuclear rms charge radii. High-energy electron scattering [53–56, 64, 65], and μ -mesic X-rays [66] have been used to obtain rms radii throughout the periodic table. The experimental proton rms radii extracted from Coulomb energies [63], from electron scattering [65], and from μ -mesic X-rays [66] have been used to construct Fig. 26 which compares these values with the proton rms radius calculated with respect to the c.m. in the HF model. The values calculated here therefore do not include the radius of the c.m. nor that of the proton internal charge distribution. The relation between the point proton distribution rms

radius $\langle r_p^2 \rangle^{1/2}$ and the charge rms radius $\langle r_{ch}^2 \rangle^{1/2}$ was taken to be, as usual,

$$\langle r_p^2 \rangle = \langle r_{ch}^2 \rangle - 0.64, \quad \text{in } F^2, \quad (3.6)$$

where $0.64 F^2$ is the mean-square charge radius of the proton itself. The experimental points and their error bars were obtained by error weighted averages of all data available for a given nucleus and errors of $\pm 0.1 F$ were assigned arbitrarily to any given datum when not quoted explicitly. The light broken lines are the computed values and the heavy line represents the $A^{1/3}$ law. Although the agreement between theory and experiment is generally good, notable discrepancies for ${}^6\text{Li}$, the oxygen isotopes, and the nuclides with $A \geq 32$, can be observed. These cases will now be discussed.

Suelzle *et al.* [67] were able to fit the e^- -scattering data on ${}^6\text{Li}$ by using a form factor

$$F(q^2) \propto \exp[-a_1^2 q^2] - a_2^2 q^2 \exp[-a_2^2 q^2], \quad (3.7)$$

corresponding to a proton distribution radius of $2.40 \pm 0.05 F$, but could not find a simple shell model wavefunction which would account for that form; on the other hand the ${}^7\text{Li}$ data was readily fitted using simple wavefunctions, thus indicating difficulties in the ${}^6\text{Li}$ structure analysis. Other experiments, involving particle transfer reactions, indeed led to the conclusion that the wavefunction of ${}^6\text{Li}$ should include sizeable ${}^3\text{He}$ - ${}^3\text{H}$ [68], and α - d [69] cluster components. A fit of the e^- - ${}^6\text{Li}$ data using wavefunctions projected from deformed and α - d cluster Slater determinants [70] gave the values 2.22 and 2.27 F , respectively, for the proton distribution radius. These calculated results lie in between our present value and the experimental point. This plus the fact that ${}^6\text{Li}$ is particularly underbound in Fig. 6, and Table II, suggests that the SD is especially inadequate in representing the correct wavefunctions of odd-odd, light $N = Z$ nuclei.

It will be noticed in Fig. 26, that the present calculation accounts nicely for the nearly constant [63] proton radii in the region $7 \leq A \leq 15$. Indeed our results seem to overemphasize this effect and carry it to the oxygen isotopes whereas the data show a definite break at ${}^{16}\text{O}$. The experimental situation appears to be well in hand in the oxygen region [71] so that we must conclude, as in Subsection D, that an additional effect, perhaps vibrations (see the discussion), is required in order to improve agreement with experiment. A similar flattening of the proton radius dependence in the region $32 \leq A \leq 40$ is predicted and not observed. Here the Nilsson model and experiment quite unambiguously suggest the occurrence of well-developed vibrational modes [72], so that the present behavior of our static intrinsic states may be a normal consequence of the HF approximation.

A close examination of Fig. 26 and Table II will reveal that in many cases the rms proton radius of an isotope is predicted to decrease as the atomic mass number

is increased. However, scarcity of data with sufficient accuracy and our difficulties with the absolute values of some of the rms radii preclude a detailed comparison of our predictions with the observed radii at this time.

F. Intrinsic Quadrupole Moments

Most of the intrinsic states obtained in this work are not spherically symmetric and some are even nonaxial. A general description of the charge quadrupole ellipsoid is obtained by computing the three quantities

$$\langle r_i^2 \rangle = \langle \Psi_0 | \sum_{n=1}^z (r_i^n)^2 | \Psi_0 \rangle, \quad i = 1, 2, 3, \quad (3.8)$$

which characterize the proton quadratic moments along each of the intrinsic coordinate axes, in the principal coordinate system. Whenever the intrinsic state generates a rotational band, these quantities can be related to experimentally observed transition and static electric quadrupole moments of the various members of the band, provided the collective dynamics is known. Short of performing exact projection, something outside the scope of this work, we shall assume that this dynamics is given by the familiar rotational model [73]. The rotational dynamics of axial intrinsic states is relatively simple since the collective angular momentum is perpendicular to the symmetry axis. The situation for nonaxial states such as ^{24}Mg , which has the ratios 1.00: 0.69: 1.88 for the moments of Eq. (3.8), and ^{32}S , for which these ratios are 1.00: 0.78: 0.46, is more complicated. Following Davydov and Filippov [74] we shall make the simplifying assumption that even those rotational bands have a good value of angular momentum projection along the intrinsic z axis, which is furthermore assumed to be the one for which the intrinsic quadrupole moment has the largest absolute value (see below).

These assumptions allow us to write the well-known equation

$$Q_s(J, K) = [3K^2 - J(J+1)] / [(J+1)(2J+3)] Q_0, \quad K \neq \frac{1}{2}, 1, \quad (3.9)$$

for the static quadrupole moment of a state with angular momentum J belonging to a band with angular momentum projection K along the intrinsic axis, in terms of the intrinsic quadrupole moment Q_0 :

$$Q_0 = [2\langle r_3^2 \rangle - \langle r_1^2 \rangle - \langle r_2^2 \rangle]. \quad (3.10)$$

The transition moment within a K band is also related to Q_0 by

$$B(E2; i \rightarrow f) = (5e^2/16\pi) Q_0^2 \langle J_i, 2, K, 0 | J_f, K \rangle, \quad K \neq \frac{1}{2}. \quad (3.11)$$

The values of Q_0 obtained from measurements of $B(E2)$ and Q_s inside the $K=0$ rotational band of several even-even nuclei are given in Table V [75]. The discre-

TABLE V
Static Quadrupole Moments and $B(E2)$ Values for Light Even-Even Nuclei

Nucleus	Level (MeV, J^π)	$Q_0(2^+)$ (barns)	$Q_0 = -3.5Q_s$ (barns)	$B(E2)^\dagger(e^2b^2)$ $\Gamma(\text{eV})$ or $\tau(\text{s})$	$ Q_0 = 3.17 \sqrt{B E 2^\ddagger}$ (barns)
^{12}C	4.43, 2^+			$0.0117 \pm 0.0009 \text{ eV}^b$ $5.64 \pm 0.4 \times 10^{-14} \text{ s}$	0.205 ± 0.013
^{16}O	$6.06, 0_2^{+a}$ $\rightarrow 6.92, 2_1^{+}$			$1.4 \pm 0.5 \times 10^{-5} \text{ eV}^c$ $470 \times 10^{-8} \text{ s}$	0.417
^{20}Ne	1.63, 2^+	-0.27 ± 0.10^d -0.26 ± 0.05^e	$+0.94 \pm 0.35^d$ $+0.91 \pm 0.18$	$17.7 \pm 2.6 W \cdot U.^d$	0.54 ± 0.02^d
^{24}Mg	1.36, 2^+	-0.243 ± 0.035^f -0.26 ± 0.08^g	$+0.85 \pm 0.12^f$ $+0.91 \pm 0.28$	$20 W \cdot U. \pm 10 \%^f$	0.65 ± 0.05^f
^{28}Si	1.78, 2^+	$+0.11 \pm 0.05^e$ $+0.17 \pm 0.05^f$	-0.39 ± 0.18 -0.59 ± 0.18	$0.72 \pm 0.04 \times 10^{-12} \text{ s}^f$	0.56 ± 0.04^f
^{32}S	2.23, 2^+	-0.20 ± 0.06^e	$+0.70 \pm 0.21$	$0.033 \pm 0.005 e^2 b^2^e$	0.58 ± 0.04
^{36}Ar	1.97, 2^+			$0.4 \pm 0.1 \times 10^{-12} \text{ s}^h$ $0.5 \pm 0.11 \times 10^{-12} \text{ s}^i$	0.59 ± 0.06 0.52 ± 0.06

^a all $E2$ transitions are from g.s. to 2_1^{+} , except in ^{16}O , as indicated;
^b Ref. [76]; ^c Ref. [77]; ^d Ref. [78]; ^e Ref. [79]; ^f Ref. [80]; ^g Ref. [81]; ^h Ref. [82]; ⁱ Ref. [83].

pancy of about 30% which is noticed there, between the values of Q_0 extracted from Q_s , and those extracted from $B(E2)$ is quite puzzling. Recent large-scale shell model calculations [84] do not account for such effects. We have pointed out in Subsection D that the presence of large hexadecapole moments in the intrinsic state might well affect the experimental determination of Q_s . For this reason we shall not consider further the data extracted from Q_s . The values of Q_0 extracted from $B(E2)$ are compared with the Q_0 calculated from Eqs. (3.8) and (3.10) and our HF wavefunctions, in Fig. 27. The diamond points in that figure are values compiled from spectroscopic moments information [79], and may be less reliable due to uncertainties in the atomic fields. As mentioned earlier, for a nonaxial state the value of Q_0 depends on the choice made of the intrinsic z axis. In Fig. 27

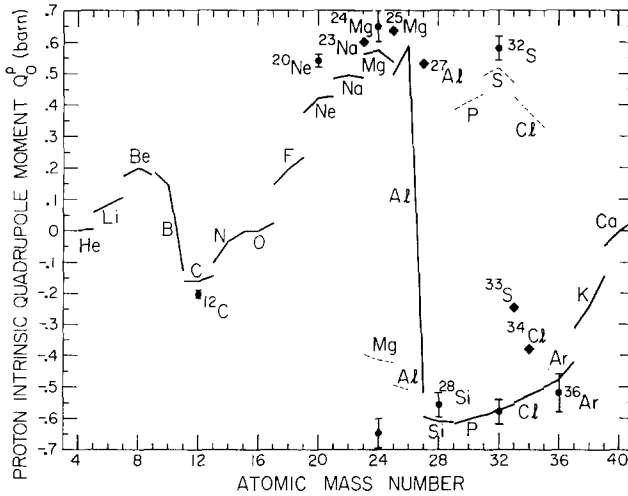


FIG. 27. Calculated and experimentally deduced intrinsic quadrupole moments for protons. Data points with error bars are those listed in Table V deduced from $B(E2)$ values. The diamonds are from Ref. [78, 79]. The dashed lines show the quadrupole moments with the second largest absolute values for the highly axially asymmetric states.

the calculated Q_0 which has the second largest absolute value (dashed line) for each highly axially asymmetric state is also shown. It is noticed that in each of these cases the two absolute values of Q_0 are not very different.

In addition to the data presented in Fig. 27, we may compare the value 0.42 barns for the Q_0 of the 6.06 MeV rotational band in ^{16}O , given in Table V, with our value 0.57 barns for the intrinsic state labelled $^{16}\text{O}^*$ in Table II. No $B(E2)$'s have so far been measured in the $^{12}\text{C}^*$ (7.65 MeV) band whereas we predict 0.71 barns for that intrinsic moment. It is clear that a more critical assessment of our

ability to reproduce quadrupole moments will require that angular momentum projection be carried out. Figure 27 indicates generally good agreement considering the severe approximations involved. It is also notable that the HF values of β_p and γ_p are generally similar to β_0 , γ_0 , those predicted in the Nilsson model (see Table II). According to Banerjee *et al.* [85] this predominance of the kinetic energy term in determining the equilibrium deformation is related to the large ratio of central to tensor components and the relatively short-range nature of the effective N - N interaction.

G. Proton-Neutron rms Radii Differences

The broken charge symmetry of the nuclear wavefunction, which results from the presence of the Coulomb interaction, is of great interest since, among other things, its quantitative explanation constitutes a good test of our knowledge of these wavefunctions and of the methods of perturbation theory used to compute the symmetry breaking. The differences in the rms radii $r = \langle r^2 \rangle^{1/2}$ of the proton and neutron distributions, due to the Coulomb interaction, for nuclei with $N = Z$ and $N = Z \pm 1$, constitute an excellent example of charge symmetry breaking and will be discussed in this section.

We first consider the even-even and odd-odd nuclei for which $N = Z$, where the effect of the charge asymmetry on the radii is well described by the normalised radii differences $\delta = (r_p - r_n)/r_p$. The computation of δ from our wavefunctions involves the relation $Ar_i^2 = Zr_p^2 + Nr_n^2$ from which r_n may be extracted from the c.m. r_p and r_i given in Table II. The values of δ are displayed in Fig. 28, as a function of $A^{1/3}$. The simple empirical expression

$$\delta \left(N = Z = \frac{A}{2} \right) \cong 0.004A^{1/3} - 0.003 \quad (3.11)$$

was used to plot the solid line through the individually calculated values. The lower line constitutes the prediction of the refined liquid drop or "Droplet" model of Myers and Swiatecki [86], and is seen to account for only about 1/3 of the differences computed here. The restrictions imposed by our truncated basis are not expected to be responsible for the discrepancy since a larger basis should allow the protons to expand further *outward*, if need be, and might thus *increase* the computed values of δ , but not decrease them as would be required to improve agreement. Of course, it may simply be that the number of nucleons is too small for the statistical properties of the droplet model to hold. Here we shall outline a simple calculation which appears to account for a much large fraction of the observed shift.

We write the total binding energy as the sum of a Coulomb term W_c (coming from the two-body v_c alone) and a nuclear term W_N (everything in W except W_c).

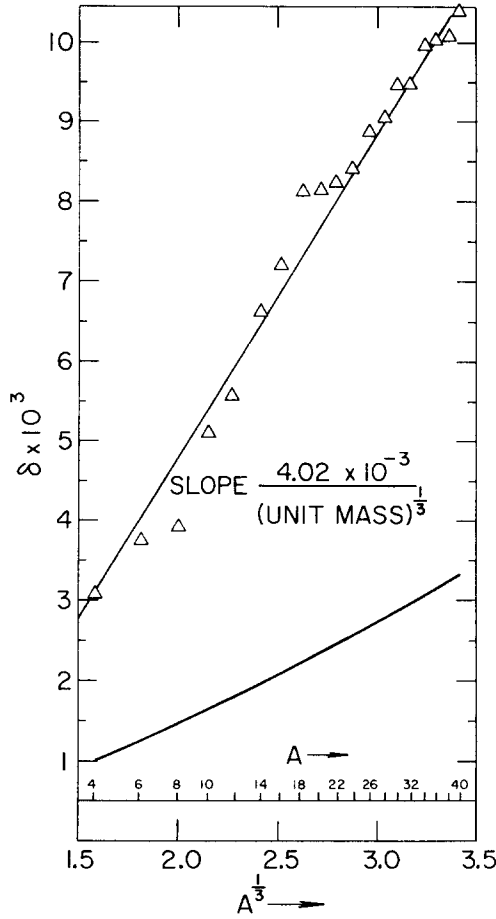


FIG. 28. Predicted value for $\delta = (r_p - r_n)/r_p$ for $N = Z$ nuclei. The heavy line is calculated from the formula derived in the droplet model [86]. The thin line is a guide through the HF results.

The total energy can be expanded [87], to second order, in a power series of the fractional perturbations δ_p and δ_n , about its equilibrium value $W^0 = W_N^0$ ($r_p = r_n$, $\delta_p = \delta_n = 0$), when the Coulomb interaction is turned off.

$$W(\delta_p, \delta_n) = W_N^0 + W_c^0 (1 - \delta_p) + \frac{1}{8} K A (\delta_p + \delta_n)^2. \quad (3.12)$$

K is the nuclear matter compressibility coefficient, and the Coulomb terms comes from assuming a uniformly distributed charge. The two parameters δ_p and δ_n are not independent of each other, due to the symmetry energy term not explicitly

shown here. We choose to eliminate the spurious degree of freedom by defining the ratio, $\gamma = \delta_n/\delta_p$, with the expectation that γ should be mass independent, to first order, at least for $N = Z$ nuclei. This is borne out by performing separate HF calculations, with v_c excluded from the Hamiltonian, for ^{16}O , ^{28}Si and ^{40}Ca . The values for γ , with a mean of 0.43, for these nuclei are shown in Table VI.

TABLE VI
Effects of the Coulomb interaction on the rms radii^a

	(a)		(b)				$\Delta = (b) - (a)$				$\gamma^{(1)}$	γ
	$r^{(1)}$	r	$r_p^{(1)}$	$r_p^{(1)}$	r_p	r_n	$\Delta_n^{(1)}$	$\Delta_n^{(1)}$	Δ_n	Δ_n		
^{16}O	2.369	2.317	2.398	2.381	2.345	2.329	0.029	0.012	0.028	0.012	0.42	0.43
^{28}Si	2.938	2.910	2.978	2.955	2.949	2.927	0.040	0.017	0.039	0.056	0.43	0.42
^{40}Ca	2.103	3.082	3.165	3.131	3.144	3.110	0.062	0.028	0.062	0.028	0.45	0.45

^a $r^{(1)}$ is sp rms radius. r is the rms radius with respect to the c.m. Columns under the headings (a) and (b), respectively, list the radii calculated without and with the Coulomb interaction included in the Hamiltonian, respectively. γ is the ratio Δ_n/Δ_p .

W can now be expressed in terms of the quantity, $\delta = \delta_p - \delta_n$, we are presently interested in.

$$W(\delta) = W_N^0 - [W_c^0/(1 - \gamma)]\delta + \frac{1}{8}KA[(1 + \gamma)/(1 - \gamma)](\delta^2). \quad (3.13)$$

The stability condition, $\partial W/\partial \delta = 0$, then leads to the relation

$$\delta = 4W_c^0/KA[(1 - \gamma)/(1 + \gamma)^2]. \quad (3.14)$$

Using a value of $K = 200$ MeV, the Coulomb energies listed in Table II for W_c^0 (any reasonable value for W_c^0 will suffice the present purpose), and $\gamma = 0.43$, we obtain the values for $\delta \times 10^3$ of 5.2, 8.0 and 10.7, respectively, for ^{16}O , ^{28}Si and ^{40}Ca , to be compared with the values 7.26, 9.0 and 10.4 shown in Fig. 28. Although it is clear that the results obtained from (3.14) are not entirely independent of the HF results, we have nevertheless shown that the gross feature of the proton-neutron radius differences calculated in HF can be understood in rather simple terms.

We now turn to the matter of the proton-neutron radii differences for the proton rich and neutron rich nuclei of Table II. We denote by $N_+(Z_+)$ the neutron (proton) rich member of the approximate $T = \frac{1}{2}$ isospin-doublet mirror nuclei. To begin with, one observes that for the N_+ nuclei, r_p and r_n are similar, indicating a somewhat higher neutron density, while for the Z_+ nuclei, r_p is appreciably greater than

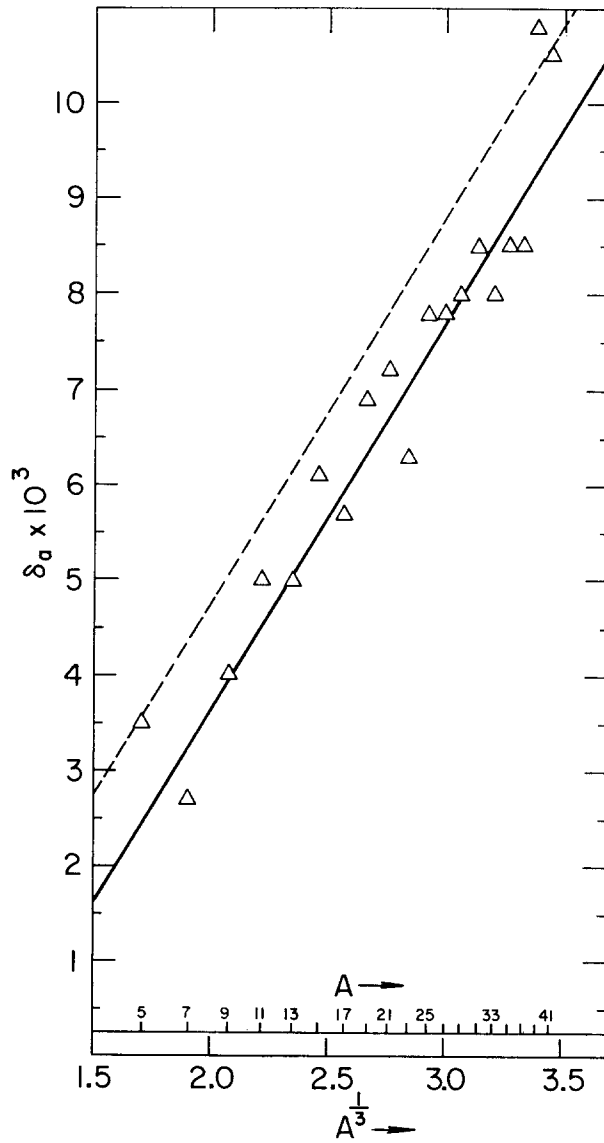


FIG. 29. Calculated mean values of δ (see text) for $|N - Z| = 1$ nuclei. The dashed line is a reproduction of the thin line in Fig. 29.

r_n . This is indeed as intuition would have it concerning the interplay of a strong p - n force, a weaker n - n force and still weaker p - p force, but it does complicate the matter of extracting the effects of the Coulomb force on the radii differences. For example, the usual quantities, $r_p(Z_+) - r_n(Z_+)$ and $r_p(N_+) - r_n(N_+)$ tell us mostly that we have an unequal number of protons and neutrons and say little about the additional radii differences induced by the charge asymmetry. We shall therefore consider mixed differences of the form

$$\delta(N_+) = \frac{1}{r_t(N_+)} [r_p(N_+) - r_n(Z_+)], \quad (3.15a)$$

$$\delta(Z_+) = \frac{1}{r_t(Z_+)} [r_p(Z_+) - r_n(N_+)]. \quad (3.15b)$$

They would vanish in the absence of Coulomb interaction and so they do measure the effect of interest here.

To simplify the presentation we display only the mean, $\delta_a = \frac{1}{2}(\delta(N_+) + \delta(Z_+))$, in Fig. 29. Individually, $\delta(N_+)$ and $\delta(Z_+)$ can readily be extracted from Table II. The solid line in Fig. 29 obeys the fitting equation

$$\delta_a(A) = 0.004A^{1/3} - 0.004, \quad |N - Z| = 1, \quad (3.16)$$

and the dashed line is the fitting equation (3.11) of Fig. 28. The systematics of the proton-neutron radius differences shown in this section are quite regular and we eagerly await the appearance of experimental data for comparison.

H. Coulomb Energies

Perhaps the most direct experimental manifestation of the charge asymmetry of nuclear states is the differences ΔE_c in binding energies between the members of $T = \frac{1}{2}$ isospin doublets. These plus many other related energy comparisons have been intensely studied in the past and have been reviewed recently by Janecke [88] and by Nolen and Schiffer [89]. Here we shall discuss these properties in the ground states of the nuclei in Table II.

The first difference of the binding energies of $T = \frac{1}{2}$ mirror nuclei is called the the Coulomb displacement energy $\Delta E_c(Z)$ and we compute it as

$$\begin{aligned} \Delta E_c(Z) &= W(Z+1, N) - W(Z, N+1) \\ &= W(Z_+) - W(N_+), \quad N = Z, \end{aligned} \quad (3.17)$$

using the HF binding energies W of Table II. These values are compared with experimental ones in Fig. 30. The empirical data reasonably well reproduced by the calculation, including the shell effect at $A = 16$. Yet, the calculated values are seen to fall slightly below experiment for $A \geq 27$ and the shell effect at $A = 40$

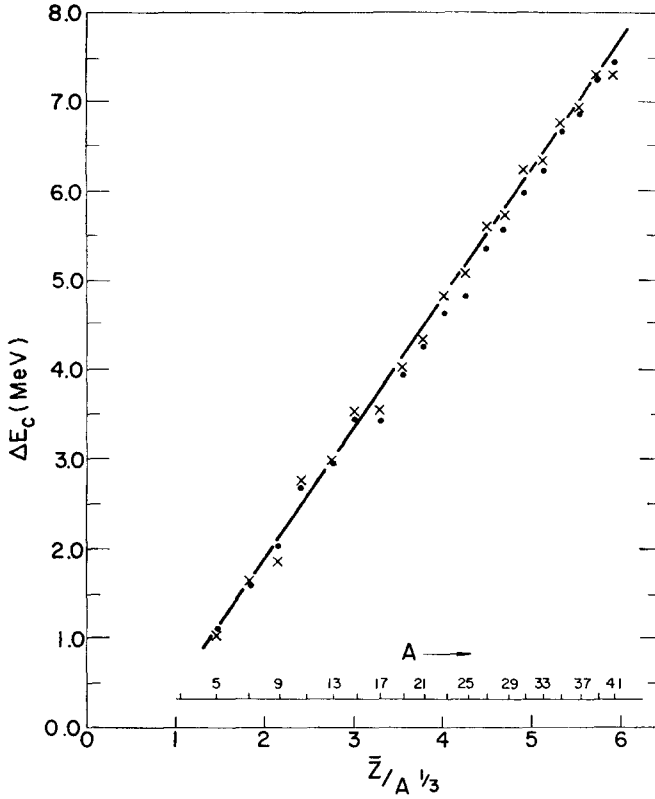


FIG. 30. Calculated (·) and experimental (×) Coulomb displacement energies. The line shows the two-parameter fit [88] $\Delta E_c = 1.430 Z A^{-1/3} - 0.992$ (MeV). Z is the mean proton number.

is not reproduced. The latter effect can be understood in terms of the basis limitation. It is known that ΔE_c is strongly dominated by the rms radius of proton distribution and since the predicted r_p are too small for the heavier nuclei the discrepancy between the predicted ΔE_c and the experiment value is actually larger than that appeared in Fig. 30 for these nuclei. The odd-even or pairing effect observed in Fig. 30 is best studied by considering the second differences $\Delta^2 E_c(Z)$ defined as

$$\Delta^2 E_c(Z) = \Delta E_c(Z) - \Delta E_c(Z - 1). \quad (3.18)$$

It can be seen from Fig. 30 that the second difference is large for odd Z and small for even Z . The jump is related to Δ_g , the Coulomb pairing energy defined as

$$\Delta_g(Z) = \frac{1}{2}[\Delta^2 E_c(Z + 1) - \Delta^2 E_c(Z)], \quad Z \text{ even}, \quad (3.19a)$$

$$= \frac{1}{2}[\Delta^2 E_c(Z) - \Delta^2 E_c(Z + 1)], \quad Z \text{ odd}. \quad (3.19b)$$

The mean experimental value [88] of Δ_g is ~ 180 keV in the p -shell and ~ 130 keV in the s - d shell whereas we obtain a mean of ~ 95 keV in both shells. The discrepancy is perhaps not too surprising since explicit pair correlations have not been considered here. We have seen earlier that our T -violating method accounts for most but not all of the pairing energy, and the residual pairing energy may have some effect on Δ_g . The value of Δ_g was calculated by Carlson and Talmi [90], in the j - j coupling scheme and for $10 \leq Z \leq 14$, to be ~ 110 keV. In the more sophisticated seniority scheme of Hecht [91] the values 108, 87, and 76 keV were obtained in the $0p_{3/2}$, $0d_{5/2}$ and $0d_{3/2}$ shells, respectively [92]. These calculations then also fail to account for the full value of Δ_g ; they do include pairing correlations but treat the Coulomb interaction to first order and are not self-consistent. We expect the combined pairing and self-consistent effects to be sufficient to account for all of the observed Δ_g .

The HF method offers the unique opportunity to find out how much of the Coulomb displacement energy comes from changes in the nuclear energy due to the charge asymmetry in the wavefunction. We separate the total Hamiltonian into its nuclear and Coulomb components $H = H_N + V_c$ and compute separately $W_N = \langle \psi_0 | H_N | \psi_0 \rangle$ and $W_c = \langle \psi_0 | V_c | \psi_0 \rangle$, where $|\psi_0\rangle$ is the self-consistent state obtained by iterating with the full Hamiltonian, as explained in Section II. Both $W = W_c + W_N$ and W_c are given in Table II. Thus we write

$$\Delta E_c^0(Z) = W_c(Z_+) - W_c(N_+), \quad (3.20a)$$

$$\Delta E_c^1(Z) = W_N(Z_+) - W_N(N_+), \quad (2.20b)$$

ΔE_c^1 is the quantity of interest and $\Delta E_c(Z)$ is now given by

$$\Delta E_c(Z) = \Delta E_c^0(Z) + \Delta E_c^1(Z). \quad (3.21)$$

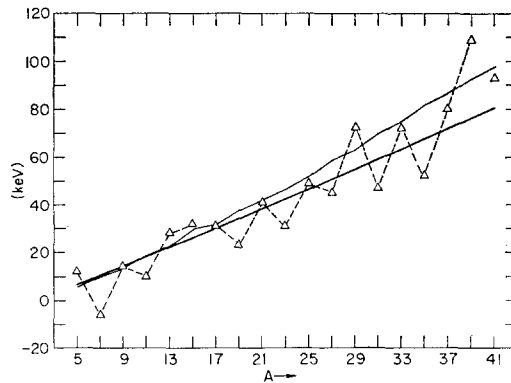


FIG. 31. The correction $\Delta E_c^1 = \Delta E_c - \Delta E_c^0$. The thin line is calculated from Eq. (3.22), the dark line from (3.23). The triangles are calculated in the HF approximation.

ΔE_c^1 is easily extracted from Table II. The results are shown (triangles) in Fig. 31. Again these results can be understood in simple terms. Expressed in terms of the fractional proton-neutron radius difference and using Eq. (3.11), taken at $A = 2Z$, we have, to first order,

$$\begin{aligned}\Delta E_c^1 &= W_c(Z_+) \delta(Z_+) - W_c(N_+) \delta(N_+) \\ &\equiv W_c(Z_+) [0.004(A+1)^{1/3} - 0.003] - W_c(N_+) [0.004(A-1)^{1/3} - 0.003]\end{aligned}\quad (3.22)$$

This fitting formulas is further simplified by using the uniformly charged sphere for approximation $(3e^2/5r) Z^2 A^{-1/3}$ for W_c ,

$$\Delta E_c^1 \cong \frac{1}{r_0} (3.2A - 2.6A^{2/3})(\text{keV}), \quad r_0 = 1.3. \quad (3.23)$$

The values of ΔE_c^1 from the last two equations are also shown in Fig. 31 and they agree with the HF result. It is seen that for the heavier nuclei ΔE_c^1 is of the order of 100 keV and therefore cannot be ignored in any detailed calculation of the Coulomb displacement energy.

Whenever the wavefunction can be expressed as a single SD , as is the case here, it is interesting to separate the total Coulomb energy W_c in two terms

$$W_c = W_{cD} + W_{cE}, \quad (3.24)$$

where W_{cD} is the direct term

$$W_{cD} = \frac{e^2}{2} \int d^3\mathbf{x} \int d^3\mathbf{x}' \rho_p(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho_p(\mathbf{x}'), \quad (3.25)$$

and W_{cE} is the exchange term,

$$W_{cE} = - \frac{e^2}{2} \int d^3\mathbf{x} \int d^3\mathbf{x}' |\rho_p(\mathbf{x}, \mathbf{x}')|^2 \frac{1}{|\mathbf{x} - \mathbf{x}'|}; \quad (3.26)$$

we note that Eq. (2.28) has been used to define $\rho_p(\mathbf{x}, \mathbf{x}')$ and $\rho_p(\mathbf{x}) = \rho_p(\mathbf{x}, \mathbf{x})$. The direct term W_{cD} does have a classical limit and may thus be estimated in the simple model of a uniform spherical charge distribution of radius $R = r_0 A^{1/3}$ to yield the well-known expression

$$W_{cD} = (3e^2/5r_0)(Z^2/A^{1/3}). \quad (3.27)$$

On the other hand, the mixed or off-diagonal density $\rho_p(\mathbf{x}, \mathbf{x}')$ does not have any classical counterpart and a knowledge of the wavefunction is required to obtain it.

In the statistical model of Bethe and Bacher [62] the proton sp states are assumed to be plane waves normalised in a cubic box of equivalent volume, with side $l = [4\pi/3]^{1/3}R$. This yields the expression

$$W_{cE} \cong -\frac{3}{4}\alpha(e^2/r_0)(Z^{4/3}/A^{1/3}), \quad \alpha = [3/2\pi]^{2/3}, \quad (3.28)$$

so that the normalized ratio $-Z^{2/3}W_{cE}/W_{cD}$ is constant and equal to 0.76 in this model. We have compared this estimate with the predictions of the HF calculation, for the $N = Z$ nuclei, in Table VII. The direct and exchange components of W_c

TABLE VII

Values for the normalised ratio $-W_{cE}/W_{cD} \times Z^{2/3}$, calculated in the HF approximation, for $N = Z$ nuclei, to be compared with the statistical model prediction of $5/4 (3/2\pi)^{2/3} = 0.76$.

Z	ratio	Z	ratio
2	0.792	12	0.752
3	0.806	13	0.748
4	0.820	14	0.746
5	0.791	15	0.741
6	0.772	16	0.741
7	0.743	17	0.735
8	0.740	18	0.733
9	0.744	19	0.728
10	0.749	20	0.716
11	0.747		

are not given separately here but were obtained in the course of the calculation. It will be seen that the agreement is surprisingly good considering the simplicity of the model; the HF results are within $\pm 6\%$ of the statistical model in the region $2 \leq Z \leq 20$.

We next examine the contributions of the direct and exchange terms to the Coulomb displacement energies, Eq. (3.17), for $T = \frac{1}{2}$ mirror nuclei pairs, by computing the usual percentage exchange factor

$$\epsilon(Z) = -100[\Delta E_{cE}(Z)/\Delta E_{cD}(Z)], \quad (3.29)$$

where ΔE_{cE} and ΔE_{cD} are defined as in Eq. (3.17) but using W_{cE} and W_{cD} , respectively. The predictions of the statistical model for this quantity are obtained via Eqs. (3.27) and (3.28), as

$$\epsilon(Z) = 51Z^{-2/3}[1 - (1/3Z) + \mathcal{O}(1/Z^2)]. \quad (3.30)$$

It would also be of interest to compare our results for ϵ with the predictions of shell model perturbation theory calculations. There one assumes that for the extra

proton outside a closed j shell nucleus, namely ^{12}C , ^{16}O , ^{28}Si and ^{40}Ca , the Coulomb displacement energy may be represented as arising from the interaction of the odd proton with the core protons. This results mostly in a neglect of the self-energy contributions to the direct part of ΔE_c . The statistical model may still be used to define a new exchange factor $\epsilon'(Z)$ in the absence of self-energies as

$$\epsilon'(Z) = 100[\alpha Z^{1/3}(1 + (1/6Z)) - (3/5)]/(6/5)Z. \quad (3.31)$$

The quantity is not easily obtained directly in the HF model so we produce a hybrid estimate as follows: We suppose that the Z dependence of ϵ' in the HF calculation is similar to that of Eq. (3.31), and that the most important difference from the statistical model comes from the numerical constant α which characterises the plane wave equivalent volume. Using Eqs. (3.27) and (3.28), Eq. (3.30) is rewritten as an explicit function of α , which is then chosen to make that equation agree with Eq. (3.29), the HF prediction for $\epsilon(Z)$. These values of α are then used in Eq. (3.31) to obtain the corrected value of ϵ' . The results of this exercise are shown in Table VIII which compares the values of ϵ' obtained with the statistical model value

TABLE VIII
The Exchange Factor ϵ' (%)

Z	A	Statistical theory $\epsilon'(\alpha = 0.61)$	"Hartree-Fock" α	ϵ'	Shell ^a Model
2	5	9.7	0.58	8.0	
3	7	9.1	0.58	7.9	
4	9	8.5	0.52	5.4	
5	11	8.0	0.52	5.3	
6	13	7.5	0.51	4.9	6.7
7	15	7.1	0.53	5.2	
8	17	6.7	0.51	4.6	5.4
9	19	6.4	0.54	5.0	
10	21	6.1	0.53	4.7	
11	23	5.9	0.54	4.8	
12	25	5.7	0.52	4.2	
13	27	5.5	0.56	4.7	
14	29	5.3	0.52	4.0	3.8
15	31	5.1	0.51	3.7	
16	33	5.0	0.52	3.8	4.4
17	35	4.8	0.52	3.7	
18	37	4.7	0.51	3.5	
19	39	4.6	0.52	3.5	
20	41	4.4	0.53	3.5	3.7

^a Ref. [89].

of α , those obtained with the HF corrected values of α and shell model values [89] $A = 13, 17, 29$ and 41 . The various results for ϵ and ϵ' are summarised in Fig. 32.

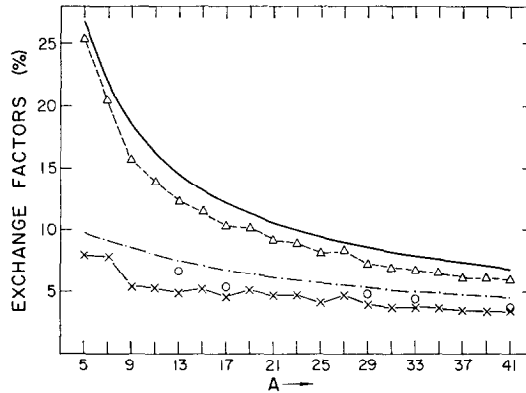


FIG. 32. Exchange factors ϵ (direct term includes Coulomb self-energy) and ϵ' (direct term does not include Coulomb self-energy). The solid line is ϵ predicted by the statistical expression of Bethe and Bacher [62], the triangles are calculated in the HF approximation, the dot-dashed line is ϵ' predicted by the statistical expression, the crosses are ϵ' obtained in the HF approximation, and the open circles are ϵ' calculated in the shell model in first order perturbation [89] theory.

The solid line is given by the statistical model Eq. (3.30) for ϵ while the triangles are computed directly from the HF results by using Eq. (3.29). The dot-dash line represents the statistical expression Eq. (3.31) for ϵ' , while for the crosses the same expression is used with the HF modified values of α ; finally, the circles represent the shell model values of Table VIII.

The agreement is good considering the approximations made. In particular, it will be noticed that the statistical model expressions for W_{cD} and W_{cE} contain no Coulomb pairing terms so that they would predict $\Delta_g = 0$ when substituted in Eq. (3.19). It has been proposed [92] that a pairing term be added to W_{cE} in the statistical model, in order to account for Δ_g . The effect of this in Fig. 32 would be to change the smooth statistical curve for ϵ' to a broken one which would fluctuate from about 3.5% (A even) to about 10% (A odd). This does not seem to agree with our result. From the basis of the present work it may be concluded that the contribution to Δ_g comes from *both* W_{cD} and W_{cE} but not from the latter alone.

H. Isospin Impurities

The presence of isospin vectors and tensors in the Coulomb Hamiltonian implies that the true eigenfunctions of the N, Z nuclear system will contain

components [93] with $|(N - Z)/2| \leq T \leq |(N + Z)/2|$ where T is the total isospin of a nuclear state, and where it is assumed that both the proton and the neutron are exactly the $T = \frac{1}{2}$ members of an isospin doublet. The possible internal violation of isospin for p and n due to their Coulomb self-interaction is a much higher energy particle-physics phenomenon which can not reasonably be covered in the present context. An interesting experimental consequence of the isospin mixing discussed above led Anderson and Wong [94] to the discovery of isobaric analog states for heavier nuclei; since then a great many experiments and calculations have been performed to study isospin impurities, some of which have been reviewed recently by Soper [95].

Our purpose here will be to compute the expectation value $\langle T^2 \rangle = \langle \Psi_0 | T^2 | \Psi_0 \rangle$, of the total isospin squared, on the HF wavefunction obtained in the presence of v_c . We have

$$T^2 = \sum_{n=1}^A |\tau_n|^2 + \sum_{n \neq n'} \tau_n \cdot \tau_{n'}, \quad (3.32)$$

in the usual notation, as a separation of T^2 into 1- and 2-body components. Recalling that our sp wavefunctions do not mix neutrons and protons, it is not difficult to reduce the expectation value of Eq. (3.32) to the expression

$$\langle \Psi_0 | T^2 | \Psi_0 \rangle = \frac{1}{4}(N - Z)^2 + \frac{1}{2}(N + Z) - \text{Tr}[\rho^p \rho^n], \quad (3.33)$$

where ρ^p and ρ^n are the proton and neutron density matrices, and the trace of their product is given by

$$\text{Tr}[\rho^p \rho^n] = \sum_{i,j} \left| \int \phi_i^{*p}(\mathbf{x}) \phi_j^n(\mathbf{x}) d^3\mathbf{x} \right|^2, \quad (3.34)$$

in the HF basis; the sum is over all occupied proton states i , and all occupied neutron states j . This expression simplifies considerably if $|\Psi_0\rangle$ is invariant under the exchange of proton and neutron orbits, and reduces to

$$\text{Tr}[\rho^p \rho^n] = \min(N, Z), \quad (3.35)$$

so that we then have $\langle T^2 \rangle = T_0(T_0 + 1)$, $T_0 \equiv |T_Z| = \frac{1}{2}|N - Z|$. In the absence of symmetry between neutron and proton orbits the overlaps of Eq. (3.34) can only decrease and Eq. (3.33) then shows that $\langle T^2 \rangle$ will be increased. The symmetry of $|\Psi_0\rangle$ with respect to exchange of neutron and proton orbitals depends not only on the symmetries of the Hamiltonian but also on the symmetries of the initial trial wavefunction, as pointed out in Section 2. Thus even in the absence of Coulomb forces the HF state of an $N \neq Z$ nucleus will not have the required symmetry because the initial wavefunction does not have it. This additional isospin

deformation of the intrinsic state is therefore a spurious consequence of the method of calculation. For example, it has recently been estimated by Brink and Svenne [96], under somewhat restrictive assumptions, to be about 10 % of the true mixing induced by the Coulomb interaction in ^{48}Ca . The removal of the spurious mixing for $N \neq Z$ should involve additional ground state correlations as introduced by RPA calculations [97]. We shall deal mostly with $N = Z$ nuclei here so that the spurious mixing will not be our main concern.

We calculate the isospin impurity in the following manner: We first consider the expansion of $|\psi_0\rangle$, which has good T_z , on a basis of states $|T, T_z\rangle$ which have also good total T , that is

$$|\Psi_0(T_z)\rangle = a_0 |T_0, T_z\rangle + a_1 |T_0 + 1, T_z\rangle + \dots, \quad (3.36)$$

where $\sum_i a_i^2 = 1$. We truncate the sum at $T = T_0 + 1$ in order that $\langle T^2 \rangle$ above may be used. This will give us an upper bound for P the percentage impurity of the $T_0 + 1$ component as

$$P = 100a_1^2 = 100[\langle T^2 \rangle - T_0(T_0 + 1)]/2(T_0 + 1). \quad (3.37)$$

The $N = Z$ results of this calculation are given in Fig. 33 and are compared with

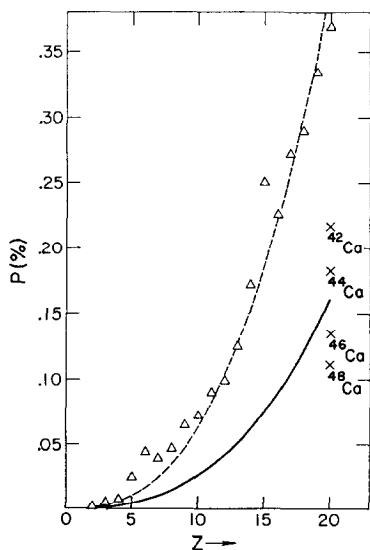


FIG. 33. Isospin impurities for the ground state of $N = Z$ nuclei. The triangles are HF results, the solid line is the prediction of Bohr *et al.* [98] and the dashed line represents 2.5 times the impurity of their prediction. The crosses are the HF predictions of the impurities for the ground states some $N > Z$, even calcium isotopes.

the predictions (solid line) of Bohr *et al.* [97], based on collective model arguments, and parametrised by

$$P = 5.55 \times 10^{-5} Z^{8/3} \quad (N = Z). \quad (3.38)$$

The dotted line through the HF points represents the same equation as above but with the constant taken as 13.1×10^{-5} , which is some 2.5 times larger than the value of Bohr *et al.* We also show in Fig. 33 our calculated isospin impurities for ^{42}Ca , ^{44}Ca , ^{46}Ca , and ^{48}Ca ; these numbers and the other results we now discuss in the shell-model and collective model perturbation theory context.

Soper [95] has estimated P , using shell model perturbation theory to be 1.8 % for ^{40}Ca and 0.15 % for ^{48}Ca . Thus a considerable discrepancy is found between the three calculations. Perhaps the only similarity between the present and other methods is the rough agreement we find with the $Z^{8/3}$ dependence predicted by the collective model. The decrease in P observed here in going from ^{40}Ca to ^{48}Ca is due almost entirely to what Soper calls the geometric quenching effect arising from the rapid increase of the denominator in Eq. (3.37) while the numerator remains relatively constant. For example, the pure geometric quenching implied by maintaining the numerator at its ^{40}Ca value would predict 0.18, 0.12, 0.09, and 0.07 % for $^{42-48}\text{Ca}$ whereas we observe 0.22, 0.18, 0.15, and 0.11 % for this series of isotopes.

Amongst the other sources of quenching [95, 98] which strongly and critically affect the perturbation calculations of P , the analog quenching mechanism whereby a large splitting between $T = T_0$ and $T = T_0 + 1$ particle hole states is induced, plays a dominant role via the energy denominators involved. No such effect is involved explicitly here but we must recognize that ground state correlations induced by zero-point vibrations in isospin space, as implied by the term F_{pnpn} of Eq. (2.22d), an effect which is completely neglected here, could significantly alter our predictions for the isospin mixing percentage P .

VI. SUMMARY AND DISCUSSION

Many of the ground state properties of some 57 light nuclei have been calculated in the HF approximation, by using a semirealistic two-body nucleon–nucleon reaction matrix with no other empirical parameter, and compared with available experimental data as well as with results predicted by other theoretical methods. It has been shown that several of these properties can satisfactorily be accounted for in this model and that interesting quantitative predictions for isospin related effects can be obtained.

In particular, we have found that the empirical systematics of the total binding energies and the sp separation energies are semiquantitatively reproduced by our

results, with better agreement than had hitherto been thought possible in such a model with no density and no energy dependence in the reaction matrix. The discrepancies in those calculated quantities have been assigned to the residual rotational and pairing correlation energies which were not included in this calculation based on the intrinsic state alone. Upon restoration of rotational and time-reversal invariance, a future endeavor, for which the Hill-Wheeler generator coordinate method is well suited, it is expected that improved agreement with experiment will be obtained.

A careful examination of the density distributions of the nuclei investigated has shown that definite alpha particle structures emerge from the self-consistent iterations without being postulated at the outset, in several $N = Z$ even-even light nuclei. The alpha cluster structures observed here were found to be in reasonable agreement with those of the explicit alpha particle models, within our parity and basis restrictions. One of the better known parameters of the density distribution, the rms charge radius has been seen to agree well with experiment in the region $A \leq 32$, except for ${}^6\text{Li}$ and the oxygen isotopes, where too small values are predicted. The values predicted in the region $A > 32$ were also found to be too small. The discrepancy in ${}^6\text{Li}$ is attributed to a possible parity violating α - d cluster structure outside the reach of our calculation. The other discrepancies were speculated to occur from the necessity of imposing a size-increasing collective vibrational superstructure to the intrinsic states obtained here. The converse explanation, namely, the one where a density-dependent two-body effective interaction is constructed, which includes in the HF state the effects of vibrational correlations, is equally acceptable, notwithstanding the possible objection that these correlations might not be describable by a single SD . So striking an example has been given recently [99] of the ability of a SD to mimic the effect of the even more complicated short-range correlations in ${}^{16}\text{O}$, that we have no hesitation in making this proposal to account for the apparent differences between the approximate reaction matrix used here and the phenomenological density dependent interactions currently in use [11, 12, 100]. Furthermore, as we have seen in this paper, the pairing correlations can also be imitated quite effectively by introducing time-reversal violating components in the SD $|\psi_0\rangle$. In addition our rms charge radii calculation agrees well with experiment in predicting that the p -shell nuclei starting at ${}^8\text{Be}$ have radii greater than those predicted by the $A^{1/3}$ law and are nearly constant up to the shell closure at $A = 16$, as emphasized by Wilkinson and Mafethe [63]. Still, the accuracy and amount of experimental data available on charge rms radii is till too restricted to make any further systematic comparison at the present time. As a third important property of our density distributions, the electric intrinsic quadrupole moments have been found in most cases to agree with experiment within their errors and ambiguity of definition; the experimental intrinsic moments have been deduced through the extreme rotational model

approximation, either from the static quadrupole moments of the 2^+ member of the band, or from the $B(E2: 0^+ \rightarrow 2^+)$. We have found better agreement with the values extracted from $B(E2)$.

On the subject of the Coulomb interaction, a matter of great current interest, the present model is capable of detailed predictions. We have obtained a relation, Eq. (3.11), between r_p and r_n the rms proton and neutron radii of the $N = Z \leq 20$ nuclei which we reproduce here, for convenience, in a slightly different form as

$$r_p - r_n \cong (0.004A^{1/3} - 0.003) r_p, \quad N = Z \leq 20. \quad (3.11)$$

It was somewhat surprising to find that this difference is nearly three times that predicted by the droplet model of Myer and Swiatecki [86] since their calculation, unlike ours, does not suffer from basis restrictions which might decrease the computed values of $r_p - r_n$. This was taken as evidence that our basis is adequate, for the nuclei considered, in reproducing most of the effects of the Coulomb repulsion, perhaps with the exception of the $A = 41$ nuclei where anomalous wavefunctions might imply sizeable admixtures of $N = 5$ major shell states, states which are mostly outside our basis. We have made calculations with and without Coulomb interaction and confirmed that the Coulomb force expands *both* the proton *and* the neutron densities, the neutrons being dragged along nearly half as far out as the protons by the strong neutron-proton attractive nuclear force. This information has allowed us to obtain rather good fits to our complex numerical calculation with extremely simple models which had been thought in the past to have only qualitative validity [Eq. (3.14)]. Although the present results may not be reliably extrapolated to heavy nuclei where a considerable neutron excess is present, we see that the highly neutron rich isotopes of the light nuclei can easily be studied with the aim of deriving extrapolation formulas for the heavier ones. These results will be reported elsewhere. The situation for the $T = \frac{1}{2}$ mirror nuclei, with $Z_+(N_+)$ denoting the proton (neutron) rich member, was also found to be interesting. Whereas we have the relations $r_n(Z_+) = r_p(N_+) < r_n(N_+) = r_p(Z_+)$ in the absence of Coulomb interaction, we have confirmed the intuitive prediction that the proton radii in both the above equalities are greater than the neutron ones when the repulsive Coulomb force is turned on. It is appropriate here to emphasize that the proton and neutron density distributions in mirror nuclei are different enough that one should view with considerable skepticism arguments which make liberal use of charge symmetry properties to simplify otherwise intractable perturbation calculation of charge symmetry violation effects. Our work also suggests that for heavier nuclei where significant neutron excesses are present, it is not reasonable to assume that the protons and the core neutrons have the same rms radii.

The systematics of Coulomb energies were analysed in some detail and emphasis

was put on the experimentally observable Coulomb displacement energies ΔE_c , calculated as total binding energy differences between approximate isobaric analog states. Here we were restricted to $T = \frac{1}{2}$ pairs. We found that our calculated values did exhibit the observed shell discontinuity at ^{16}O ; we were also able to account for about 50 and 70% of the Coulomb pairing energy observed in the p and $s - d$ shells, respectively, although as mentioned earlier, no explicit pair correlations are involved in the present single SD model. Apart from explicit pairing correlations, which might increase Δ_σ , we note that the spin-orbit term in the two-body Coulomb interaction could significantly affect Δ_σ , being of order 100 keV in the light nuclei [89]. This term was neglected here because of its very small effect on the total binding energy. The structure of ΔE_c was probed further by decomposing it first into a component directly related to the Coulomb potential ΔE_c^0 and a component ΔE_c^1 due to the action of the nuclear force on the Coulomb perturbed wavefunctions. A new numerical expression which fits the calculated results, Eq. (3.23), was given for ΔE_c^1 . It predicts the value $\Delta E_c^1 = +90$ keV for the ^{41}Ca - ^{41}Sc pair. We have also seen in Eq. (3.22) that the positive sign was related to the repulsive nature of the Coulomb force and the resulting *increase* of the proton radius over the neutron radius. For a hypothetical attractive long-range perturbative interaction the sign ΔE_c^1 would, of course, still be positive since its sign only expresses the fact that the nuclear force must saturate, i.e., provide an absolute energy minimum in the absence of the perturbation. This effect was seemingly neglected in a recent analysis of the various contributions to ΔE_c^1 , by Auerbach *et al.* [101], who obtained the value $\Delta E_c^1 = -210 \pm 200$ keV, for the ^{41}Ca - ^{41}Sc pair. The largest contributions to their quoted uncertainty came from their estimate of the possible contributions of charge dependence of the nuclear force (-100 ± 100 keV) and of the short-range correlation effects ($\sim +100$ keV).

It is important not to confuse the contribution to ΔE_c^1 due to the isospin impurity P , as analyzed by Auerbach *et al.*, with the correlation ΔE_c^1 calculated in this work. In the former, the correction is formulated such that it is proportional [101] to $-P$. Therefore, it is always less than zero. On the other hand we have seen that the isospin impurity results from an increase in the proton radius which, in turn, implies an *increase* in ΔE_c^1 . The relation between P and ΔE_c^1 is further complicated by the fact that ΔE_c^1 is a measure of the increase in the *total* radius, as caused by the Coulomb repulsion, whereas P measures only the *difference* between proton and neutron radii increases. Table VI shows that the strong proton-neutron interaction forces the neutron distribution to expand half as much as does the proton distribution when the Coulomb interaction is turned on.

To summarize the situation regarding our results for ΔE_c , we may say that after renormalizing our values to account for the differences between the calculated and experimental charge radii, they remain too small by 100 to 400 keV. These

discrepancies may be explained in terms of systematic radius anomalies [89], or they may be due to small differences in the correlations induced by residual nuclear and Coulomb interactions [102]. The second possibility is clearly favored over the first one by this work.

A second decomposition of ΔE_c in terms of a direct and exchange term was performed and showed that the statistical model of Bethe and Bacher [62] overestimated the ratio of exchange to direct term by only some 15 to 20 %. Generally good agreements with shell-model perturbation theory was obtained for this exchange ratio. We have also found that the statistical model agreed with our estimate of the exchange to direct ratio of the total Coulomb energy to within 6 %. Thus this model could be useful in fission problems where small corrections to the Coulomb energy could change the delicate equilibrium between the nuclear binding energy and the Coulomb energy and thus affect calculations of the fission potential barrier [103].

Finally, the isospin impurities of the ground states of the $N = Z$ nuclides were computed under the plausible assumption that the predominant impurities are $T = 1$ components, and were found to be nearly 2.5 times larger than those predicted in the collective model [98] but nearly 4 times smaller than the shell-model prediction [95] in the case of ^{40}Ca . However, it was pointed out that the presence of ground state correlations might affect the values obtained here. Indeed, recent calculations by Mohan *et al.* [104] support this expectation.

The main conclusion of this work is now clear; it appears that one can indeed account quantitatively for many of the ground state properties of the light nuclei by using a unique, energy-independent, density-independent two-body semi-realistic interaction. Using the methods outlined here and described further elsewhere [24] it is well within the power of present-day computing facilities to increase the basis size to include up to 186 protons and 186 neutron orbits, especially if the J sum in Eq. (2.13) is truncated around the 5- multipole component of F . Thus similar calculations can clearly be conducted for most of the nuclei in the periodic table. The problem of projection will be treated elsewhere. Here we need only mention that a suitable adaptation of the method of "cross-state" density matrices of Löwdin [1] to the discrete approximation of the Hill-Wheeler generator coordinate method, appears to be well suited for the matter of projecting from such a large basis. Furthermore, improved methods for generating the initial trial wavefunction, perhaps as cluster wavefunctions, would greatly enhance the power of the HF method. Finally, it is hoped that the present results will be viewed as a challenge to deduce from first principles the most appropriate form for the nuclear effective interaction to be used in this type of calculation.

ACKNOWLEDGMENTS

We are most grateful to G. Saunier and B. Rouben who calculated all the SP2 elements used here. We also wish to thank T. K. Alexander and O. Häuser who provided the data compilation on quadrupole moments, J. C. Hardy for illuminating comments on Coulomb energies, and M. Harvey, F. C. Khanna and A. Jensen for fruitful discussions. Finally, our gratitude goes to D. McPherson and the staff of the Mathematics and Computation Branch for their active cooperation in the complex numerical calculations involved here.

REFERENCES

1. P. O. LÖWDIN, *Phys. Rev.* **97** (1955), 1474.
2. D. R. HARTREE, *Proc. Cambridge Phil. Soc.* **24** (1928), 89.
3. V. I. FOCK, *Z. Phys.* **61** (1930), 126.
4. K. A. BRUECKNER, A. M. LOCKETT, AND M. ROTENBERG, *Phys. Rev.* **121** (1961), 255.
5. K. T. R. DAVIES AND M. BARANGER, *Phys. Rev. C* **1** (1970), 1640.
6. R. J. MCCARTHY AND K. T. R. DAVIES, *Phys. Rev. C* **1** (1970), 1640.
7. M. K. PAL AND A. P. STAMP, *Phys. Rev.* **158** (1967), 924.
8. G. RIPKA, in "Advances in Nuclear Physics," (M. Baranger and E. Vogt, Eds.), Vol. 1, Plenum Press, New York, 1968, and references therein.
9. M. R. GUNYE, *Nucl. Phys. A* **118** (1968), 174.
10. D. R. TIERPE, W. H. BASSICHIS, AND A. K. KERMAN, *Nucl. Phys. A* **142** (1970), 49; W. H. BASSICHIS, A. K. KERMAN, AND J. P. SVENNE, *Phys. Rev.* **160** (1967), 746.
11. J. W. NEGELE, *Phys. Rev. C* **1** (1970), 1260.
12. D. VAUTHERIN AND D. M. BRINK, C. N. R. S. Report IPNO/TH180; D. VAUTHERIN AND M. VENERONI, *Phys. Lett. B* **29** (1969), 203.
13. C. W. NESTOR, K. T. R. DAVIES, S. J. KRIEGER, AND M. BARANGER, *Nucl. Phys. A* **113** (1968), 14; R. M. TARBUTTON AND K. T. R. DAVIES, *Nucl. Phys. A* **120** (1968), 1.
14. G. SAUNIER AND J. M. PEARSON, *Phys. Rev. C* **1** (1970), 1353.
15. T. T. S. KUO, in the "Fourth Symposium on Low-Medium Mass Nuclei," University of Kansas, Oct. 1970, to be published.
16. J. EICHLER AND A. FAESSLER, *Nucl. Phys. A* **157** (1970), 166; D. M. BRINK, H. FRIEDRICH, A. WEIGUNY, AND C. W. WONG, *Phys. Lett. B* **33** (1970), 143.
17. B. GIRAUD AND P. U. SAUER, *Nucl. Phys. A* **154** (1970), 587.
18. B. R. MOTTelson, in "The Many Body Problem," Les Houches Summer School in Theoretical Physics, Wiley, New York, 1958.
19. R. Y. CUSSON, "ELMOS — A CDC-6600 Fortran IV Code to Manipulate Single Particle Wavefunctions and solve the Ellipsoidal Modified Oscillator Problem," Atomic Energy of Canada Ltd., Chalk River, Ontario, AECL report no. 3730 (1970).
20. S. G. NILSSON, *Mat. Fys. Medd. Dan. Vid. Selsk.* **29** (1955), No. 16.
21. R. Y. CUSSON, unpublished.
22. R. M. DREIZLER, F. R. KREIS, AND A. KLEIN, *Nucl. Phys. A* **155** (1970), 33, and references therein.
23. J. D. TALMAN, *Nucl. Phys. A* **141** (1970), 273.
24. R. Y. CUSSON AND H. C. LEE, "EVALIN — A CDC-6600 Fortran IV Code to Perform an Extended Variational Approximation for Light and Intermediate Nuclei," Atomic Energy of Canada Ltd., Chalk River, Ontario, AECL report no. 3801 (1970).

25. F. VILLARS, Course 23, Proc. Int. School of Physics "Enrico Fermi," Academic Press, New York, 1963; Course 36, Proc. Int. School of Physics "Enrico Fermi," Academic Press, New York, 1966; M. BARANGER, "Cargese Lectures in Theoretical Physics" (M. Levy, Ed.), Benjamin, New York, 1963.
26. D. J. THOULESS, *Nucl. Phys.* **21** (1960), 225.
27. D. J. THOULESS, *Nucl. Phys.* **22** (1961), 78.
28. We reserve the roman indices $i, l, m, \dots$, for sp states in the HF basis, and the greek indices $\alpha, \beta, \gamma, \dots$, for states in the expansion basis of Table I.
29. A. JENSEN AND M. HARVEY, private communication, 1970.
30. W. H. BASSICHIS, B. A. POHL, AND A. K. KERMAN, *Nucl. Phys. A* **112** (1968), 360.
31. M. BARANGER, *Phys. Rev.* **120** (1960), 957; **122** (1961), 992.
32. D. M. BRINK AND G. R. SATCHLER, "Angular Momentum," 2nd ed. Clarendon Press, Oxford, 1969.
33. M. HARVEY, in "Advances in Nuclear Physics," (M. Baranger and E. Vogt, Eds.), Vol. 1, Plenum Press, New York 1968.
34. I. TALMI, *Helv. Phys. Acta* **25** (1952), 185; M. MOSHINSKY, *Nucl. Phys.* **13** (1959), 104.
35. E. P. WIGNER, "Group Theory and its Application to the Quantum Mechanics of Atomic Spectra," Academic Press, New York, 1959.
36. A. M. LANE, "Nuclear Theory," Benjamin, New York, 1964.
37. M. BARANGER, *Nucl. Phys. A* **149** (1970), 225; J. ARPONEN, *Nucl. Phys. A* **155** (1970), 597; A. N. JAMES, in "Proceedings of the International Conference on Properties of Nuclear States," (M. Harvey et al., Eds.), University of Montreal Press, Montreal, 1969.
38. N. M. HUGENHOLTZ AND L. VAN HOVE, *Physica* **24** (1958), 363.
39. We are most grateful to Dr. Saunier and Dr. Rouben, who kindly calculated all the G -matrix elements of SP2 and SP3 used in this work.
40. R. A. BRYAN AND B. L. SCOTT, *Phys. Rev. B* **135** (1964), 434.
41. S. KAHANA, H. C. LEE AND C. K. SCOTT, *Phys. Rev.* **185** (1969), 1378.
42. C. SHAKIN, Y. R. WAGHMARE AND M. H. HULL, *Phys. Rev.* **161** (1967), 1006; **161** (1967), 1015.
43. K. E. LASSILA, M. H. HULL, JR., H. M. RIPPEL, F. A. McDONALD, AND G. BREIT, *Phys. Rev.* **126** (1962), 884.
44. P. FEDERMAN, B. GIRAUD, AND D. ZAIKIN, *Nucl. Phys. A* **102** (1967), 81; W. H. BASSICHIS AND L. WILLETS, *Phys. Rev. Lett.* **22** (1969), 799, and references therein.
45. J. BAR-TOUV AND I. KELSON, *Phys. Rev.* **138** (1965), B1035.
46. S. GOSHEN AND H. J. LIPKIN, *Ann. Phys.* **6** (1959), 301.
47. R. Y. CUSSON, *Nucl. Phys. A* **114** (1968), 789.
48. R. Y. CUSSON, *Can. J. Phys.* **47** (1969), 2835; R. Y. CUSSON AND B. CASTEL, *Phys. Rev. Lett.* **23** (1969), 871.
49. W. H. BASSICHIS AND L. WILLETS, *Phys. Rev. Lett.* **22** (1969), 799.
50. K. IKEDA, N. TAKIGAWA, AND H. HORIUCHI, *Supp. Prog. Theor. Phys.* Extra Number, 464 (1968).
51. J. M. E. MATTAUCH, W. THIELE, AND A. H. WAPSTRA, *Nucl. Phys.* **67** (1965), 1.
52. S. N. TEWARI AND G. L. STRUBLE, *Phys. Rev. C* **1** (1970), 1156.
53. R. HOFSTADTER, *Rev. Mod. Phys.* **28** (1956), 214.
54. H. F. EHRENBERG, R. HOFSTADTER, U. MEYER-BERKHOUT, D. G. RAVENHALL, AND S. E. SOBOTTKA, *Phys. Rev.* **113** (1959), 666.
55. J. B. BELLICARD, P. BOUNIN, R. F. FROSH, R. HOFSTADTER, J. S. MCCARTHY, F. J. UHRHANE, M. R. YEARIAN, B. C. CLARK, R. HERMAN, AND D. G. RAVENHALL, *Phys. Rev. Lett.* **19** (1967), 527.

56. R. F. FROSCH, R. HOFSTADTER, J. S. MCCARTHY, G. K. NÖLDEKE, K. J. VAN OOSTRUM, M. R. YEARIAN, B. C. CLARK, R. HERMAN, AND D. G. RAVENHALL, *Phys. Rev.* **174** (1968), 1380.
57. B. D. DAY, *Rev. Mod. Phys.* **39** (1967), 719, and references therein.
58. F. C. KHANNA, *Nucl. Phys. A* **165** (1971), 475.
59. D. M. BRINK, Course 36, Proc. Int. School of Physics "Enrico Fermi" (C. Bloch, Ed.), Academic Press, New York, 1966.
60. E. B. CARTER, G. E. MITCHELL, AND R. H. DAVIES, *Phys. Rev. B* **133** (1964), 1421.
61. D. CLINE, private communication.
62. H. A. BETHE AND R. F. BACHER, *Rev. Mod. Phys.* **8** (1936), 82.
63. D. H. WILKINSON AND M. E. MAFETHE, *Nucl. Phys.* **85** (1966), 97.
64. T. DEFOREST, JR. AND J. D. WALECKA, *Adv. in Phys. Phil. Mag. Supp.* **15** (1966), 1.
65. H. R. COLLARD, L. R. B. ELTON, AND R. HOFSTADTER, Landolt-Börnstein numerical and functional relationships in "Science and Technology," New Series, Group 1, Vol. 2, Springer-Verlag, Berlin, 1967.
66. C. S. WU AND L. WILETS, *Ann. Rev. Nucl. Sci.* **19** (1969), 527.
67. L. R. SUELZLE, M. R. YEARIAN, AND H. CRANNEL, *Phys. Rev.* **162** (1967), 992.
68. B. L. BERMAN, *Phys. Rev. Lett.* **95** (1965), 1271.
69. P. GAILLARD, *Phys. Rev. Lett.* **25** (1970), 593.
70. Y. SUZUKI AND K. KUBODERA, *Prog. Theor. Phys.* **44** (1970), 617.
71. R. P. SINGHAL, T. R. MOREIRA, AND H. S. CAPLAN, *Phys. Rev. Lett.* **24** (1970), 73; data from this reference were also incorporated in Fig. 26.
72. B. CASTEL, W. C. STEWART, AND M. HARVEY, *Nucl. Phys. A* **162** (1971), 273.
73. For an introduction to the rotational model, see M. A. PRESTON, "Physics of the Nucleus," Addison-Wesley, Reading, MA, 1962.
74. A. S. DAVYDOV AND G. F. FILIPPOV, *Nucl. Phys.* **8** (1958), 237; A. S. DAVYDOV AND V. S. ROSTOVSKY, *Nucl. Phys.* **12** (1959), 58.
75. We are indebted to T. K. ALEXANDER AND O. HÄUSER for permission to use the results of their compilation.
76. S. J. SKORKA, J. HERTEL, AND T. W. RETZ-SCHMIDT, *Nucl. Data A* **2** (1966), 347.
77. C. P. SWANN AND F. R. METZGER, *Phys. Rev.* **108** (1957), 982; J. LOWE, A. R. POLETTI, AND D. H. WILKINSON, *Phys. Rev.* **148** (1966), 1045.
78. D. SCHWALM AND B. POVH, *Phys. Lett. B* **29** (1969), 103.
79. K. NAKAI, J. L. QUÉBERT, F. S. STEPHENS, AND R. M. DIAMOND, *Phys. Rev. Lett.* **24** (1970), 903.
80. O. HÄUSER, *Phys. Rev. Lett.* **23** (1969), 320.
81. A. HAMBERGER, P. G. BIZETTI, AND B. POVH, *Phys. Rev. Lett.* **21** (1968), 1599.
82. J. P. THIBAUD, *J. de Phys.* **31** (1970), 1311.
83. H. GRAWE AND K. P. LIEB, *Nucl. Phys. A* **127** (1969), 13.
84. B. H. WILDENTHAL, J. B. MCGRORY, AND P. W. M. GLAUDEMANS, *Phys. Rev. Lett.* **26** (1971), 96.
85. M. K. BANERJEE, C. A. LEVINSON, AND G. J. STEPHENSON, JR., *Phys. Rev.* **178** (1969), 1709.
86. W. D. MYERS AND W. J. SWIATECKI, *Ann. Phys. (N.Y.)* **55** (1969), 395; W. D. MYERS, *Phys. Lett. B* **30** (1969), 451.
87. L. R. B. ELTON, "Nuclear Sizes," Oxford University Press, London, 1961.
88. J. JANECKE, in "Isospin in Nuclear Physics," (D. H. Wilkinson, Ed.), p. 297, North-Holland, Amsterdam, 1969.
89. J. A. NOLAN, JR. AND J. P. SCHIFFER, *Ann. Rev. Nucl. Sci.* **19** (1969), 471.
90. B. C. CARLSON AND I. TALMI, *Phys. Rev.* **96** (1951), 436.

91. The relation $A_g = (8/3)(2j + 1)c$, was used, where the c 's are Hecht's values, quoted by Jänecke in Ref. [88].
92. S. SENGUPTA, *Nucl. Phys.* **21** (1960), 542.
93. Thus *effective* Coulomb interactions may contain third and higher order tensor components; see G. G. BERTSCH AND S. KAHANA, *Phys. Rev. Lett. B* **33** (1970), 193.
94. J. D. ANDERSON AND C. WONG, *Phys. Rev. Lett.* **7** (1961), 350.
95. J. M. SOPER, in "Isospin in Nuclear Physics," (D. H. Wilkinson, Ed.), North-Holland, Amsterdam, 1969.
96. D. M. BRINK AND J. P. SVENNE, *Nucl. Phys. A* **154** (1970), 449.
97. C. A. ENGELBRECHT AND R. H. LEMMER, *Phys. Rev. Lett.* **24** (1970), 607.
98. A. BOHR, J. DAMGAARD AND B. R. MOTTelson, in "Nuclear Structure" (A. Hossain, H.-ar-Rashid and M. Islam, Eds.), North-Holland, Amsterdam, 1968.
99. T. W. DONNELLY AND G. E. WALKER, *Phys. Rev. Lett.* **22** (1969), 1121.
100. J. ZOFKA AND G. RIPKA, C.E.N.S. Report, submitted to *Nucl. Phys.*
101. N. AUERBACH, J. HÜFNER, A. K. KERMAN AND C. M. SHAKIN, *Phys. Rev. Lett.* **23** (1969), 484.
102. E. AUERBACH, S. KAHAN, C. K. SCOTT, AND J. WENESER, JR., in "Nuclear Isospin," Proc. Conf. on Nuclear Isospin, Asilomar, 1969 (J. D. Anderson, S. D. Bloom, J. Cerny and W. W. True, Eds.), Academic Press, New York, 1969.
103. V. M. STRUTINSKY, *Nucl. Phys. A* **95** (1967), 420; S. G. NILSSON, J. R. NIX, A. SOBICZEWSKI, Z. SZYMAŃSKI, S. WYCECH, C. GUSTAFSON, AND P. MÖLLER, *Nucl. Phys. A* **115** (1968), 545.
104. R. MOHAN, M. DANOS, AND L. C. BIEDENHARN, *Phys. Rev. C* **3** (1971), 468.