PHYSICAL REVIEW C VOLUME 9, NUMBER 6 JUNE 1974

Nuclear-structure calculations with the modified Yale potential for the $2s$-$1d$ shell

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(Received 19 November 1973)

Employing the unitary-model approach of Shakin, Waghmare, Tomaselli, and Hull, and a modified version of the Yale potential, adjusted to yield a lower percentage of the "D" state in the deuteron ground state without affecting the other two-nucleon quantities calculable from the Yale potential, the ground-state properties of the even-even $N=Z$ nuclei are calculated for the $2s$-$1d$ shell by using the Hartree-Fock self-consistent approach. The healing distance for the relative $^3S_1$ state is not used as a parameter since healing is "naturally" achieved for this state. Using the same values of the oscillator and level-shift parameters, the modified Yale interaction with its reduced tensor force component yields binding energies, single-particle energies, rms radii, and deformations which are generally closer to the experimental values than those reported for the Yale potential.

[NUCLEAR STRUCTURE ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}A, ^{40}Ca; calculated single-particle energies, ground-state energies, rms radii, and ground-state deformations. Hartree-Fock method. Modified Yale interaction.]

I. INTRODUCTION

In recent years several structure calculations for the $2s$-$1d$ shell nuclei employing realistic nucleon-nucleon potentials with different core structures have been reported in the literature. Pal and Stamp[1] and Stamp[2] have used the hard-core Yale potential for performing the Hartree-Fock calculations for the $N=Z$ nuclei for $8 \leq A \leq 40$ with various oscillator parameter strengths. More recently Nisley and Hull[3] have employed the Yale[4] and Reid[5] soft-core two-body interactions to carry out calculations for the same nuclei. In calculating the effective two-body interactions, Nisley and Hull employed the unitary-model operator approach as first developed by Villars[6] and later refined and used in practical calculations by da Providencia and Shakin,[7] and by Shakin, Waghmare, Tomaselli, and Hull.[8-10]

The potentials employed above had been determined from the two-nucleon elastic scattering data and certain bound-state properties. It is well known that the elastic scattering data fix only the asymptotic form of the two-nucleon wave function, leaving the wave function at short distances undetermined. It therefore seems desirable to examine the sensitivity of the three- and many-nucleon systems to the short-range part of the two-nucleon potential. The problem has been studied by Haftel and Tabakin[11] by examining the binding energy of nuclear matter for exactly phase-shift-equivalent potentials generated by applying a unitary transformation to the Reid soft-core potential. The new potentials had a short-range nonlocality but reproduced exactly the two-body observables calculated with the Reid potential. It was found that potentials that are exactly equivalent in the nucleon-nucleon scattering problem may give variations of approximately 10 MeV in nuclear matter binding-energy calculations. For finite nuclei the off-shell effects for a set of phase shift equivalent potentials have been studied by Haftel, Lambert, and Sauer,[12] who found a variation of up to 2.8 MeV per particle. The phase-shift-equivalent potentials employed in the above calculations produce wave functions which have very unusual properties at short distances, e.g., in some cases the transformed wave functions are found to have extra nodes while in some others the two nucleons are found to approach each other very closely with an unexpected high probability.

It is well known that most of the widely used two-body interactions, namely, the Yale, Hamada-Johnston,[13] and Reid potentials yield a percentage admixture of the D state (P_D) to the ground state of the deuteron of about 7%. Due to uncertainties in the theory concerning the effects of meson exchange currents, this P_D is expected to be somewhere between 3.5–10%. Since the relative strengths of the central and noncentral components in the two-nucleon interaction are not well determined by the nucleon-nucleon scattering data, it should be possible to readjust the parameters of any one of the above-mentioned potentials in such a way as to affect the D-state probability while leaving unchanged the values of the other quantities calculable from the potential. This may be accomplished by decreasing the relative contri-

bution of the tensor component of the two-nucleon potential to the total potential. This has been recently done by Breit and collaborators[14] for the Yale potential (Y), and the modified Yale potential (MY) yields a D-state probability $P_D = 3.44\%$, retaining the quality of agreement of other calculable quantities almost the same as with the Yale potential. The wave functions obtained with the modified Yale potential have expected normal behavior.

It is therefore desirable to study the effect of the variation of the tensor force in the two-body interaction in the nuclear structure calculations. For the triton the sensitivity of the binding energy to P_D had been studied for the Yamaguchi separable potential by Levinger and collaborators.[15] It was found that the binding energy went from 7.94 to 9.01 MeV when P_D was changed from 7 to 4%. These calculations were carried out by adjusting the four parameters in the Yamaguchi tensor potential to fit the deuteron binding energy, the triplet effective range, the quadrupole moment, and P_D. This procedure, did not of course maintain the fit for the triplet phase parameters above the effective range region.

The present paper employs the modified Yale potential for calculating the two-body effective interaction following the unitary-model operator approach of Shakin, Waghmare, Tomaselli, and Hull. Using the matrix elements obtained in this fashion, the ground-state properties of the closed-shell nuclei ^{16}O and ^{40}Ca and deformed nuclei ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, and ^{36}A are calculated employing the self-consistent Hartree-Fock procedure. The results are then compared with the earlier calculations of Shakin *et al.* and Nisley and Hull. The general spirit of this work is to investigate the differences and similarities of the calculated quantities for the above-mentioned nuclei that arise when the MY and Y potentials are used without altering the approximations that enter the calculations. For this reason this study is not claimed to be an exhaustive one and not much emphasis will be put on seeking agreement with the available data on the binding energy, root mean square radius, single-particle energies, etc., though occasional comparisons will be made. We will also make rough comparison with recent calculations based on nonlocal separable and density-dependent interactions.

II. CALCULATION OF MATRIX ELEMENTS

The effective interaction matrix elements were calculated following the method of Shakin *et al.* The matrix elements between normalized and antisymmetrized two-body states of the type

$$\langle n_1(l_1\tfrac{1}{2})j_1, n_2(l_2\tfrac{1}{2})j_2 \,|\, V_{\text{eff}} \,|\, n_3(l_3\tfrac{1}{2})j_3, n_4(l_4\tfrac{1}{2})j_4\rangle_{JT}$$

are calculated using the modified Yale potential with oscillator parameters $b = 1.76$ and $b = 1.99$ fm.

Table I shows the healing distances d and pseudopotentials VP for the various relative states. It is important to point out that for the relative states $^1S_0$, $^3S_1$, $^3P_2$, $^1D_2$, $^3D_1$, $^3D_2$, and $^3D_3$ with the principal quantum number $n = 0$, the "healing" is achieved without introducing a pseudopotential. This "natural" healing is especially pronounced in the $^3D_1$ state since it was achieved even for the state with principal quantum number $n = 2$. For the other states the strengths of the pseudopotentials for the MY potential are comparable with those for the Y potentials. For the $^1P_1$ ($n = 0$) state, for instance, the pseudopotential strengths are 703 and 719 MeV, for the MY and Y potentials, respectively.

The importance of this natural healing is realized when one focuses attention on the relative state $^3S_1$, since it plays a paramount role in the resulting binding energies. This lack of choice amounts to essentially removing a fitted parameter, namely the healing distance of the $^3S_1$ state.

Table II exhibits the relative matrix elements for various interactions along with the oscillator

TABLE I. The healing distances and pseudopotentials of the relative states for the modified Yale interaction. The healing distance d is in Moshinsky units (1 Moshinsky unit $= \sqrt{2}$ fm). The oscillator parameter $b = 1.76$ fm.

State	$^1S_0$	$^3S_1$	$^1P_1$	$^3P_0$	$^3P_1$	$^3P_2$	$^1D_2$	$^3D_1$	$^3D_2$	$^3D_3$
d	0.769	0.616	0.700	0.701	0.701	0.617	0.611	0.454	0.680	0.616
n	Pseudopotential VP (MeV)									
0	0	0	−703	−260	−242	0	0	0	−248	0
1	−14	−24	−710	−272	−253	−10	−2	0	−252	−2
2	−30	−42	−735	−280	−259	−16	−4	0	−256	−8
3	−50	−67	−744	−292	−265	−28	−10	−20	−260	−12
4	−72	−92	−769	−298	−274	−36	−11	−50	−272	−14
5	−100	−124	−778	−308	−284	−46	−17	−80	−276	−20
6	−134	−158	−798	−324	−298	−59	−19	−100	−280	−26

parameters and healing distances used. For the oscillator parameter $b = 1.76$ fm the healing distances for the MY interaction are quite close to those for the Y interaction except for the $^3S_1$ and $^3D_1$ states. However, as the healing distance for the $^3S_1$ state for the MY interaction is decreased by over 20% as compared to that with the Yale interaction, the strength of the matrix element decreases by about 1% for the $n=0$, $n'=0$ case, increases by about 9% for the $n=0$, $n'=1$ case, and slightly decreases for the $n=1$, $n'=1$ case. For the $^3D_1$ state the MY interaction matrix elements show a slight increase over the Y matrix elements. For the oscillator parameter $b = 1.76$ fm, the MY matrix elements are in reasonable agreement with those calculated for the Y, Reid (R) and Hamada-Johnston (HJ) interactions. The matrix elements for the HJ interaction were calculated by Grillot and McManus[16] and Becker and Mackellar.[17] It may be mentioned that Grillot and McManus used a state-dependent level shift parameter Δ while the present calculations employed $\Delta = 20.0$ MeV. The $^3D_2$ state matrix element provides another example for comparison purposes of the relative strength of the matrix elements for the different interactions. Between the matrix elements for the MY and Y interactions obtained with healing distances of $0.680\sqrt{2}$ fm and $0.677\sqrt{2}$ fm, respectively, the former is in closer agreement with the matrix elements obtained with the R and HJ interactions, as obtained by independent ways. Note, however, the abnormally short healing distance in this state for the Reid interaction.

Table II also affords another very interesting comparison, in showing the dependence of the matrix elements on the oscillator parameter b. In general, the matrix elements obtained with the MY interaction with $b = 1.99$ fm are smaller than those for the smaller oscillator parameter. The ultimate test of the matrix elements is, of course, in the nuclear properties calculated by means of them.

A valuable comparison can also be made by calculating the relative matrix elements using the same healing distances and oscillator parameters for the MY and Y interactions as it will reveal the dependence of the strength of the matrix elements on the variation of the tensor force. Such a comparison is also included in Table II. For the MY and Y interactions with $b = 1.99$ fm, the matrix elements for the $^3S_1$ state show marked differences which vary from 24% for the $n=0$, $n'=0$ case to over 50% for higher values of n and n' (not shown in the table), the matrix elements obtained with the Y interactions being of greater magnitude. This increase can be understood by realizing that in order to achieve the shorter natural healing distances of the MY interaction larger pseudopotentials (−536.0 MeV for the $n=5$ node) had to be used for the Y interaction. This in turn demands that the level shift parameter Δ be increased. This is

TABLE II. Comparison of the relative matrix elements of the modified Yale interaction for two oscillator parameters with those for the Yale, Reid soft-core, and Hamada-Johnston (HJ) interactions. The healing distance d is given in Moshinsky units (M.u.).

			Modified Yale $b=1.76$ fm		Yale[a] $b=1.76$ fm		Modified Yale $b=1.99$ fm		Yale $b=1.99$ fm		Reid[b] $b=1.76$ fm		HJ[c] $b=1.76$ fm		HJ[d] $b=1.76$ fm
			d		d		d		d		d		Δ		
State	n	n'	(M.u.)	V_{eff}	(M.u.)	V_{eff}	(M.u.)	V_{eff}	(M.u.)	V_{eff}	(M.u.)	V_{eff}	(MeV)	t	t
$^1S_0$	0	0	0.769	−6.27	0.769	−6.10	0.769	−4.73	0.769	−4.64	0.752	−5.85	80	−5.97	−6.05
	0	1		−4.80		−4.59		−4.04		−3.88		−4.67		−4.73	−5.54
	1	1		−4.45		−4.04		−3.92		−3.69		−4.32	36	−4.43	−4.98
$^3S_1$	0	0	0.616	−8.52	0.800	−8.60	0.616	−6.37	0.616	−7.91	0.952	−9.16	80	−6.62	−8.87
	0	1		−7.45		−6.84		−5.98		−7.79		−8.35		−5.13	−10.44
	1	1		−7.33		−7.35		−6.15		−8.23		−8.80	36	−5.63	−9.71
$^1P_1$	0	0	0.700	0.44	0.705	1.52	0.700	0.44	0.700	0.40	0.696	1.35	58	1.76	1.55
$^3P_0$	0	0	0.701	−2.05	0.705	−2.36	0.701	−1.53	0.701	−1.53	0.752	−1.93	58	−2.14	−1.69
$^3P_1$	0	0	0.701	2.12	0.705	2.42	0.701	1.42	0.701	1.42	0.752	1.90	58	1.85	1.72
$^3P_2$	0	0	0.617	−0.81	0.613	−0.83	0.613	−0.49	0.613	−0.49	0.536	−0.77	58	−0.83	−0.91
$^1D_2$	0	0	0.661	−0.55	0.665	−0.58	0.657	−0.32	0.661	−0.32	0.712	−0.44	36	−0.50	−0.50
$^3D_1$	0	0	0.454	1.10	0.565	1.08	0.454	0.71	0.584	0.68	0.752	1.23	36	1.68	1.21
$^3D_2$	0	0	0.680	−2.16	0.677	−2.01	0.680	−1.35	0.680	−1.28	0.360	−2.19	36	−2.11	−2.14
$^3D_3$	0	0	0.616	0.03	0.693	0.05	0.616	0.02	0.616	0.02	0.696	0.36	36	0.04	−0.06
$^3S_1$-$^3D_1$	0	0		−4.50		−5.50		−3.11		−3.54		−5.29	36	−5.57	−5.51
	1	0		−1.62		−2.85		−1.39		−2.04		−2.65		−2.85	−2.64

[a] Reference 9.
[b] Reference 3.
[c] Reference 16.
[d] Reference 17.

TABLE III. Comparison of some modified Yale interaction two-body matrix elements with those of the Yale interaction for the $1p_{3/2}$, $1p_{1/2}$ states with $n_i = 2$ or 3, respectively, and $b = 1.76$ fm. The healing distances are given in Moshinsky units.

Healing distance						Modified Yale 0.616	Yale [a] 0.696
n_a	n_b	n_c	n_d	J	T	Matrix element	
2	2	2	2	0	1	−2.86	−2.57
				1	0	−2.69	−2.45
				2	1	−1.19	−1.13
				3	0	−4.24	−4.84
2	2	2	3	1	0	3.48	4.45
2	2	3	3	1	0	1.49	1.81
2	3	2	3	1	0	−5.82	−6.92
				1	1	−0.49	−0.53
				2	0	−5.34	−5.87
				2	1	−2.30	−2.23
2	3	3	3	1	0	0.76	1.39
3	3	3	3	0	1	−0.37	−0.04
				1	0	−2.67	−2.74

[a] Reference 3.

not done in an effort to keep the model parameters as nearly the same as possible. It must be mentioned at this point that the effective matrix elements of the Y interaction with $b = 1.99$ fm are not expected to yield reasonable results when used for calculating the ground-state nuclear properties because of their large magnitude. This point will be discussed further in the text.

Table III shows the comparative strengths of some selected two-body matrix elements calculated with the MY and Y interactions with $n_i = 2$ or 3 for the $1p_{3/2}$ and $1p_{1/2}$ states, respectively. The healing distance of the $^3S_1$ state for the MY interaction is smaller than that for the Y interaction by more than 11%; the values of the two-body matrix elements do not change in the same direction for all cases, although their over-all values are not radically different.

III. HARTREE-FOCK CALCULATIONS

A. Spherical nuclei

For the closed-shell nuclei ^{16}O and ^{40}Ca the Hartree-Fock (HF) calculations are performed using the single-particle orbitals expanded in the truncated space of harmonic oscillator wave functions. The bases used are

$$ns_{1/2}, np_{1/2}, np_{3/2}, \quad n = 1, 2, 3 \tag{1}$$

and

$$ns_{1/2}, np_{3/2}, np_{1/2}, nd_{5/2}, nd_{3/2}, \quad n = 1, 2, 3 . \tag{2}$$

The bases (1) and (2) were used for the calculation of the ground-state properties of ^{16}O and basis (2) was employed for the corresponding calculation of ^{40}Ca. These bases are not as extensive as used in the work of Ford, Braley, and Bar-Touv,[18] Lee and Cusson,[19] and Zofka and Ripka.[20] The effect

TABLE IV. Hartree-Fock results for ^{16}O for the modified Yale (MY) and Yale (Y) interactions for basis (1) ($ns_{1/2}, np_{3/2}, np_{1/2}, n = 1, 2, 3$) and basis (2) ($ns_{1/2}, np_{3/2}, np_{1/2}, nd_{5/2}, nd_{3/2}$, $n = 1, 2, 3$). The healing distance and the oscillator parameter are denoted by d and b, respectively.

	MY basis (1)	Y [a] basis (1)	MY basis (2)	MY basis (2)	Experiment	
b (fm)	1.76	1.76	1.76	1.99		
d (fm)	0.871	0.984	0.871	0.871		
BE/A (MeV)	−6.98	−9.80	−8.14	−6.79	−7.98 [b]	
rms radius (fm)	2.16	2.06	2.09	2.26	2.67 ± 0.03 [c]	
	Single-particle levels (MeV)					
					n [d]	p [e]
$1s_{1/2}$	−68.4	−78.7	−71.4	−61.5	−47.0	−40 ± 8
$1p_{3/2}$	−29.6	−37.0	−34.0	−28.8	−21.8	−18.4
$1p_{1/2}$	−20.5	−26.8	−24.3	−21.7	−15.7	−12.1
$1d_{5/2}$			−4.8	−3.2	−4.2	−0.6
$2s_{1/2}$	−1.0	−1.2	−2.5	−1.2	−3.2	
$1d_{3/2}$			3.9	3.2		
$1p_{1/2}$-$1p_{3/2}$ splitting	9.1	10.2	9.7	7.1	6.1	6.3
Gap Δ	19.5	25.6	19.5	18.5	11.5 [f]	

[a] Reference 3.
[b] Reference 23.
[c] Reference 24.
[d] Reference 25.
[e] Reference 26.
[f] Reference 27.

of using truncated single-particle bases had been earlier investigated by the Massachusetts Institute of Technology group.[21,22] However, as mentioned in the Introduction, our main object is to compare our results with those of Stamp, Shakin *et al.*, and Nisley and Hull who had also used these very bases in their calculations, and look for the differences and similarities in the results.

Table IV shows the results for the Hartree-Fock calculations for ^{16}O carried out with the MY potential with $b = 1.76$ fm and compares them with the results obtained with the Y interaction and the experimental values.[23-29] The healing distance of the $^3S_1$ state is $0.616\sqrt{2}$ fm for the MY interaction and $0.696\sqrt{2}$ fm for the Y interaction. The binding energy per nucleon for the MY interaction is less than that of the Y interaction by about 17% and is in better agreement with the experimental value. The corresponding rms radius though still considerably smaller is in better agreement as well. The MY interaction also gives better values for the single-particle energy levels, energy gap, and the $1p_{1/2}$-$1p_{3/2}$ splitting.

Table IV lends itself to a valuable comparison of the results of the HF calculation for ^{16}O for two oscillator parameters, $b = 1.76$ and 1.99 fm. It is known that the oscillator parameter which minimizes the binding energy for ^{16}O is in the neighborhood of 1.76 fm. On the other hand, calculations with $b = 1.99$ fm yield better agreement for the rms radius and the energy gap. The single-particle basis used in this case is the expanded basis given by (2). Some further improvement in the binding energy is possible by employing a still larger basis and by varying the oscillator parameter appropriately. However, this is not attempted here.

The results of the HF calculation for ^{40}Ca are shown in Table V. The expanded basis given by Eq. (2) is used and the comparison is made to the results obtained with the Y potential employing same values of the oscillator parameter and healing distance. The MY binding is −12.94 MeV per nucleon and the Yale −20.06 MeV. The MY single-particle energies for the two lowest orbitals are 20–25 MeV higher than those of the Y potential, but are still twice as deep as the experimental values, while the unoccupied levels are underbound. The disparity between the MY and Y results are solely the effect of the variation of the tensor force and thus lend to a valuable comparison. Closer agreement with experiments can be obtained by increasing the oscillator parameter and the expansion basis.

The inferiority of the MY results in comparison with the R results, also listed in Table V, may be understood in terms of a relatively short "natural" healing distance for the $^3S_1$ state for the MY interaction. The difference in the oscillator parameter may also account for some of the overbinding with the MY potential. In addition a better choice of Δ (i.e., larger Δ) would decrease the size of the effective matrix elements which in turn would result in improved values of the binding energy for ^{40}Ca. This, however, was not done as it lies outside the scope of this paper.

The binding energies in Tables IV and V neglect the center of mass and Coulomb energies, which can be estimated by simple expressions

$$E_{\text{Coul}} = 3Z(Z-1)e^2/5R\,, \quad R = 1.3A^{1/3}\ \text{fm}\,, \tag{3}$$

and

$$E_{\text{c.m.}} = -\tfrac{3}{4}\hbar\omega\,. \tag{4}$$

These corrections amount to an over-all reduction of the binding energy per nucleon by 0.27 MeV for ^{16}O and 1.67 MeV for ^{40}Ca.

All in all, the MY interaction with natural healing for the $^3S_1$ state yields better HF results for ^{16}O than those obtained with the Y interaction. The HF results for ^{40}Ca obtained with the MY interaction are inferior to those for the R interaction with a much larger healing distance for the $^3S_1$ state. The effect of decreasing the tensor force is to decrease the binding energy per nucleon for ^{40}Ca sig-

TABLE V. Comparison of the Hartree-Fock results for ^{40}Ca for the modified Yale ($b = 1.99$ fm), Yale ($b = 1.99$ fm), and Reid ($b = 2.09$ fm) interactions. The single-particle expansion basis consists of the states $ns_{1/2}$, $np_{1/2}$, $np_{3/2}$, $nd_{5/2}$, $nd_{3/2}$, $n = 1, 2, 3$. Experimental references are given in Table IV.

	Modified Yale	Yale	Reid [a]	Experiment	
d (Moshinsky units)	0.616	0.616	0.952		
d (fm)	0.871	0.871	1.346		
BE/A (MeV)	−12.94	−20.06	−11.23	−8.55	
rms radius (fm)	2.64	2.60	2.80	3.52	
Single-particle levels (MeV)				n	p
$1s_{1/2}$	−110.3	−137.3	−96.5		−50 ± 11
$1p_{3/2}$	−74.7	−95.8	−64.6		−34 ± 6
$1p_{1/2}$	−68.3	−88.7	−60.5		
$1d_{5/2}$	−41.2	−55.5	−34.2	−22.8	−15.5
$2s_{1/2}$	−30.5	−38.0	−25.0	−18.4	−10.9
$1d_{3/2}$	−29.7	−42.5	−26.7	−15.8	−8.3
$2p_{3/2}$	−6.0	−8.9	−3.4		
$2p_{1/2}$	−3.5	−6.0	−1.8		
$1p_{1/2}$-$1p_{3/2}$ splitting	6.4	7.0	4.1		
$1d_{3/2}$-$1d_{5/2}$ splitting	11.5	13.0	7.5	7.0	
Gap Δ	23.7	33.6	23.3	7.3	

[a] Reference 3.

TABLE VI. Hartree-Fock minima for ^{20}Ne. The oscillator parameter $b = 1.76$ fm. The single-particle energies are given in MeV.

	Spherical	Oblate	Oblate	Prolate	Experiment
BE/A (MeV)	−5.78	−5.82	−5.66	−6.13	−8.03 [a]
β	0.00	−0.183	−0.194	0.391	0.87 [b]
γ	0	0	0	0	
rms radius (fm)	2.783	2.774	2.745	2.752	2.91 [c]
			Single-particle levels		
$1s_{1/2}^{\pm 1/2}$	−56.89	−56.81	−55.48	−56.45	
$1p_{3/2}^{\pm 3/2}$	−27.04	−27.94	−28.61	−25.45	−19, −18 [d]
$1p_{3/2}^{\pm 1/2}$	−27.04	−26.80	−28.22	−30.97	
$1p_{1/2}^{\pm 1/2}$	−22.26	−22.28	−23.54	−22.18	−12 [d]
$1d_{5/2}^{\pm 5/2}$	−5.86	−7.03	−7.48	−3.61	
$1d_{5/2}^{\pm 3/2}$	−5.86	−5.82	−6.98	−6.52	
$1d_{5/2}^{\pm 1/2}$	−5.86	−4.50	−4.23	−12.68	
$2s_{1/2}^{\pm 1/2}$	−8.25	−8.89	−7.17	−4.77	
$1d_{3/2}^{\pm 3/2}$	−0.87	−1.85	−2.99	0.92	
$1d_{3/2}^{\pm 1/2}$	−0.87	0.16	−1.22	−2.12	
Energy gap Δ	2.39	1.86	0.31	6.16	10.11 [a]

[a] Reference 29.
[b] Reference 28.
[c] Reference 24.
[d] Reference 29.

nificantly, and by using a natural healing distance the additional parameter of the healing distance, used in fitting the calculated binding energy for $2s$-$1d$ shell nuclei, is effectively removed.

B. Deformed nuclei

The doubly even $N=Z$ deformed nuclei are treated following the procedure of Pal and Stamp. Their prescription dictates that one start with a spherical density matrix and then force asymmetry by introducing terms in the Hamiltonian, through the use of Lagrange multipliers λ_0 and λ_2. These Lagrange multipliers are expressed as functions of two parameters λ and θ.

$$\lambda_0 = \lambda \cos\theta, \tag{5}$$

$$\lambda_2 = \frac{1}{\sqrt{2}} \lambda \sin\theta. \tag{6}$$

The parameters λ and θ are then varied from −22 to +22 and 0 to 40°, respectively. Moreover, an elongation parameter β and an angle of asymmetry

TABLE VII. Hartree-Fock minima for ^{24}Mg. The oscillator parameter $b = 1.76$ fm. The single-particle energies are given in MeV. The experimental references are given in Table VI.

	Spherical	Oblate	Oblate	Prolate	Asymmetric	Experiment
BE/A (MeV)	−5.96	−5.30	−6.52	−6.64	−6.78	−8.26
β	−0.027	−0.563	−0.291	0.352	0.368	0.65
γ	0	0	0	0	19°11′	
rms radius (fm)	2.844	2.950	2.862	2.850	0.851	3.01 ± 0.03
			Single-particle levels			
$1s_{1/2}^{\pm 1/2}$	−61.72	−58.89	−63.35	−62.84	−62.54	
$1p_{3/2}^{\pm 3/2}$	−32.93	−36.19	−34.65	−29.99	−31.65	
$1p_{3/2}^{\pm 1/2}$	−32.93	−15.18	−34.20	−38.37	−37.88	
$1p_{1/2}^{\pm 1/2}$	−33.18	−35.35	−27.09	−28.58	−26.84	
$1d_{5/2}^{\pm 5/2}$	−10.35	−17.22	−12.93	−6.95	−7.77	
$1d_{5/2}^{\pm 3/2}$	−10.35	−3.10	−12.47	−11.91	−14.41	
$1d_{5/2}^{\pm 1/2}$	−10.35	4.67	−7.31	−17.80	−17.70	
$2s_{1/2}^{\pm 1/2}$	−10.29	−16.51	−14.49	−6.47	−9.10	
$1d_{3/2}^{\pm 3/2}$	−9.19	−15.39	−6.66	−3.65	−2.89	
$1d_{3/2}^{\pm 1/2}$	−9.19	−2.99	−3.59	−11.22	−5.88	
Energy gap Δ	0	0.21	0.46	0.69	5.31	9.21

TABLE VIII. Hartree-Fock minima for ^{28}Si. The oscillator parameter $b = 1.76$ fm. The single-particle energies are given in MeV. The experimental references are given in Table VI.

	Spherical	Prolate	Oblate	Experiment
BE/A (MeV)	−7.00	−7.67	−7.79	−8.45
β	−0.011	0.319	−0.324	−0.40
γ	0	0	0	
rms radius (fm)	2.914	2.921	2.925	3.08 ± 0.06
	Single-particle levels			
$1s_{1/2}^{\pm 1/2}$	−68.01	−68.19	−68.75	
$1p_{3/2}^{\pm 3/2}$	−38.41	−36.01	−42.26	−36
$1p_{3/2}^{\pm 1/2}$	−38.41	−44.54	−30.31	
$1p_{1/2}^{\pm 1/2}$	−40.87	−33.06	−40.73	−28
$1d_{5/2}^{\pm 5/2}$	−14.67	−11.46	−20.66	−17.0
$1d_{5/2}^{\pm 3/2}$	−14.67	−19.28	−10.88	
$1d_{5/2}^{\pm 1/2}$	−14.67	−22.81	−10.43	
$2s_{1/2}^{\pm 1/2}$	−14.39	−9.75	−20.26	−13
$1d_{3/2}^{\pm 3/2}$	−15.41	−7.05	−18.36	
$1d_{3/2}^{\pm 1/2}$	−15.41	−16.24	−5.69	
Energy gap Δ	0	4.78	7.48	8.69

γ are introduced which in terms of the collective coordinates are given by

$$a_0 = \beta \cos\gamma , \tag{7}$$

$$a_2 = a_{-2} = \frac{1}{\sqrt{2}} \beta \sin\gamma . \tag{8}$$

Starting with density matrices at the most apparent minima, once the energy surface for a nucleus is explored, an unconstrained Hartree-Fock calculation is initiated and the true minima in the binding energy are revealed. The single-particle states were expanded in the $2s$-$1d$ shell basis consisting of the states $1s_{1/2}$, $1p_{3/2}$, $1p_{1/2}$, $1d_{5/2}$, $2s_{1/2}$, and $1d_{3/2}$.

For ^{20}Ne, the Hartree-Fock minima are displayed in Table VI. The ground state is found to be axially symmetric with $BE/A = -6.13$ MeV. As will be discussed later, this value is about 20% better than the value obtained with the Y interaction and 5% better than the result for the R interaction. Some improvement in binding energy would result from using a still larger basis and performing angular momentum projection.

The ^{24}Mg nucleus is found to be axially asymmetric and Table VII shows the various minima for this nucleus. The minima for ^{28}Si are found in Table VIII; it shows that this nucleus is an oblate one in the ground state with a prolate solution nearby. The binding energies and other calculated parameters are substantially better than those obtained via the Y and R interaction.

An asymmetric ground state is also found for ^{32}S. Table IX shows the various minima for the eight-hole nucleus. It is interesting to note the close-lying oblate and prolate solutions for ^{32}S. For ^{36}A two sets of minima were found corresponding to two oscillator parameters. The ground-state shape for both cases is found to be oblate. The minimum for $b = 1.76$ fm yields $BE/A = -9.84$ MeV and −6.80 MeV for $b = 1.99$ fm as shown in Table X. The dependence of the results on the oscillator parameter indicates that the number of states included in the expansion should be enlarged. The last value is judged more appropriate as the oscil-

TABLE IX. Hartree-Fock minima for ^{32}S. The oscillator parameter $b = 1.76$ fm. The single-particle energies are given in MeV. The experimental references are given in Table VI.

	Spherical	Prolate	Oblate	Asymmetric	Experiment
BE/A (MeV)	−8.32	−8.50	−8.58	−8.70	−8.49
β	0.068	0.172	−0.221	−0.224	−0.37
γ	0	0	0	19°9′	
rms radius (fm)	2.984	2.971	2.977	2.975	3.23 ± 0.07
			Single-particle levels		
$1s_{1/2}^{\pm 1/2}$	−76.15	−73.89	−74.46	−74.05	≃−80
$1p_{3/2}^{\pm 3/2}$	−43.55	−42.63	−47.48	−48.21	−32
$1p_{3/2}^{\pm 1/2}$	−43.55	−47.89	−38.29	−44.79	
$1p_{1/2}^{\pm 1/2}$	−45.29	−41.74	−45.22	−37.75	−22
$1d_{5/2}^{\pm 5/2}$	−18.81	−17.27	−24.19	−25.41	−16
$1d_{5/2}^{\pm 3/2}$	−18.81	−22.67	−21.47	−23.44	
$1d_{5/2}^{\pm 1/2}$	−18.81	−24.94	−16.60	−14.68	
$2s_{1/2}^{\pm 1/2}$	−20.81	−15.60	−23.31	−21.72	−9.1
$1d_{3/2}^{\pm 3/2}$	−19.45	−15.17	−18.20	−19.22	
$1d_{3/2}^{\pm 1/2}$	−19.45	−20.82	−11.79	−10.98	
Energy gap Δ	0	1.67	1.60	4.54	6.43

TABLE X. Hartree-Fock minima for ^{36}A. The oscillator parameter $b = 1.99$ fm. The single-particle energies are given in MeV. The symbols Sp., Pr., and Ob. denote spherical, prolate, and oblate solutions, respectively. The experimental references are given in Table VI.

	$b = 1.99$			$b = 1.76$			
	Sp.	Pr.	Ob.	Sp.	Pr.	Ob.	Experiment
BE/A (MeV)	−6.59	−6.65	−6.80	−9.64	−9.70	−9.84	−8.52
β	−0.062	0.085	−0.179	−0.049	0.065	−0.135	
γ	0	0	0	0	0	0	
rms radius (fm)	3.415	3.415	3.409	3.020	3.020	3.015	
			Single-particle levels				
$1s_{1/2}{}^{\pm 1/2}$	−59.96	−59.90	−59.31	−80.34	−80.25	−79.43	
$1p_{3/2}{}^{\pm 3/2}$	−36.62	−35.72	−38.60	−49.83	−48.83	−52.03	
$1p_{3/2}{}^{\pm 1/2}$	−36.62	−38.47	−37.83	−49.83	−51.80	−50.94	
$1p_{1/2}{}^{\pm 1/2}$	−36.33	−35.26	−33.00	−48.72	−47.59	−44.96	
$1d_{5/2}{}^{\pm 5/2}$	−17.78	−16.29	−20.58	−25.01	−23.18	−28.37	−20
$1d_{5/2}{}^{\pm 3/2}$	−17.78	−18.67	−19.30	−25.01	−26.00	−26.64	
$1d_{5/2}{}^{\pm 1/2}$	−17.78	−20.02	−11.35	−25.01	−27.69	−16.54	
$2s_{1/2}{}^{\pm 1/2}$	−17.99	−16.50	−19.70	−24.92	−24.03	−27.27	
$1d_{3/2}{}^{\pm 3/2}$	−16.60	−15.35	−16.69	−22.35	−20.95	−22.47	
$1d_{3/2}{}^{\pm 1/2}$	−16.60	−17.59	−16.88	−22.35	−22.67	−23.19	
Energy gap Δ	0	0.94	5.34	0	1.72	5.93	6.48

lator parameter $b = 1.76$ fm is only fitted to give minimum binding in the neighborhood of ^{16}O.

Table XI gives an overview of the quality of the MY interaction for the four nuclei ^{20}Ne, ^{24}Mg, ^{28}Si, and ^{32}S by comparing the corresponding HF results with those of the Yale and Reid potentials and with experiments.

For ^{20}Ne the value of BE/A for the ground state is −6.13 MeV which represents an improvement over the value −5.07 MeV for the Y potential and −5.84 MeV for the R interaction; the calculated deformation parameter β is also better for the MY interaction than for the other two interactions by 10% or more. When one notes the results for ^{24}Mg and other heavier nuclei one finds that the values of the binding energies are increasingly improving for the MY potential for a high A nuclei. For ^{24}Mg, the value of BE/A is −6.78 MeV with the MY interaction and is over 22% better than the −5.54 MeV value for the Y interaction and over 6% better than the Reid interaction value of −6.37 MeV. The value obtained for the deformation parameter is also closer to the experimental value than for either of the other interactions, although it is still quite far from the experimental value. Upon further examination of this table one is convinced of the over-all improved agreement with the experimental values obtained with the MY interaction.

The results summarized in Tables IV, V, and XI do not include the center of mass and Coulomb corrections to the binding energy. These corrections can be estimated by the simple expressions (3) and (4).

IV. COMPARISON WITH OTHER CALCULATIONS

It may be desirable to compare our results with some others that have appeared in the literature in recent years. In making this comparison it should be remembered that some of these calcula-

TABLE XI. Comparison of the present results with the results of the Yale and Reid interactions for the minimum energy solutions. All the binding energies are given in MeV.

	Modified Yale			Yale [a]			Reid [b]			Experiment	
	BE/A	β	γ	BE/A	β	γ	BE/A	β	γ	BE/A	β [c]
^{20}Ne (prolate)	−6.13	0.391	0	−5.07	0.349	0	−5.84	0.356	0	−8.03	0.87
^{24}Mg (axially asymmetric)	−6.78	0.368	19°11′	−5.54	0.332	18°56′	−6.37	0.338	19°22′	−8.26	0.65
^{28}Si (oblate)	−7.79	−0.324	0	−6.35	−0.292	0	−7.24	−0.298	0	−8.45	−0.40
^{32}S (axially asymmetric)	−8.70	−0.224	19°9′	−7.11	−0.200	10°4′	−8.07	−0.208	19°13′	−8.49	−0.37

[a] Reference 2. [b] Reference 3. [c] Reference 28.

tions like those of Ford, Braley, and Bar-Touv (FBB) and Lee and Cusson employ potentials which are free from the complexities that accompany a hard-core potential in the calculation of the effective interaction. FBB employ the Tabakin interaction[30] and perform HF calculations for the deformed nuclei in the $2s$-$1d$ shell using three different model spaces. In their calculation using all orbitals up to the $1g_{9/2}$ as the basis, FBB impose the constraint that the predicted ground-state radius should equal the experimental value. This was accomplished by adjusting the oscillator length parameter in their calculation. Lee and Cusson used an expansion basis consisting of the first five

TABLE XII. Comparison of the modified Yale (MY) interaction results with those of Ford, Braley, and Bar-Touv (FBB), Lee and Cusson (LC), and Zofka and Ripka calculation I (ZR) for the density-dependent interactions of Negele (LINEG) and Brink and Boeker (B1). All the energies are given in MeV and rms radii are given in fm. The Hartree-Fock energy gap is denoted by Δ.

	MY	FBB	LC [a]	ZR (LINEG)	ZR (B1)	Experiment
^{16}O b (fm)	1.76		1.66	1.67	1.62	
Deepest level	−71.4		−64.1			~−47
Last filled level	−24.3		−21.1			~−4.2 [a]
Δ	19.5		20.6	17.9	23.1	11.53
rms radius	2.09		2.34	2.65	2.65	2.67 ± 0.03
BE/A	−8.14		−7.85	−7.94	−5.81	−7.98
^{20}Ne b (fm)	1.76	1.88	1.66	1.83	1.76	
Deepest level	−56.4	−46.1	−67.6			
Last filled level	−12.7	−7.96	−15.3			
Δ	6.2	7.03	9.7	7.2	15.1	10.11
rms radius	2.75	2.73	2.65	2.96	2.96	2.91
BE/A	−6.13	−2.00	−7.34	−7.60	−5.51	−8.03
^{24}Mg b (fm)	1.76	2.09	1.66	1.83	1.79	
Deepest level	−62.5	−44.1	−70.6			
Last filled level	−14.4	−4.56	−15.1			
Δ	5.3	1.70	8.2	5.0	12.1	9.21
rms radius	2.85	3.03	2.83	3.14	3.16	3.01 ± 0.03
BE/A	6.78	−1.70	−7.35	−7.72	−5.46	−8.26
^{28}Si b (fm)	1.76	2.09	1.66	1.83		
Deepest level	−68.8	−48.7	−75.4			
Last filled level	−18.4	−8.5	−18.6			
Δ	7.5	7.24	8.8	8.8	13.5	8.69
rms radius	2.93	3.10	2.94	3.27	3.31	3.08 ± 0.06
BE/A	−7.79	−2.19	−7.58	−8.12	−5.64	−8.45
^{32}S b (fm)	1.76	2.19	1.75	1.77	1.80	
Deepest level	−74.0	−48.95	−78.0			
Last filled level	−19.2	−6.1	−16.7			
Δ	4.5	1.02	7.7	5.0	11.1	6.43
rms radius	2.98	3.24	3.05	3.30	3.34	3.23 ± 0.07
BE/A	−8.70	−2.02	−7.71	−8.30	−5.71	−8.49
^{36}A b (fm)	1.99		1.75	1.74	1.80	
Deepest level	−59.3		−82.6			
Last filled level	−16.7		−18.3			
Δ	5.3		8.9	6.6	12.1	6.48
rms radius	3.41		3.09	3.34	3.37	
BE/A	−6.80		−8.03	−8.72	−5.95	−8.52
^{40}Ca b (fm)	1.99		1.75	1.71	1.75	
Deepest level	−110.3		−87.6			−50 ± 11
Last filled level	−29.7		−21.2			−15.8
Δ	23.7		18.4	14.4	20.5	7.27
rms radius	2.64		3.13	3.37	3.39	3.50
BE/A	−12.94		−8.44	−9.13	−6.24	−8.55

[a] The energies of the single-particle levels are those for neutrons.

major shells plus the $1h_{11/2}$ subshell and the semirealistic nucleon-nucleon interaction No. 2 of Saunier and Pearson.[31] Certainly our bases are much simpler and therefore only a rough comparison with these calculations is possible.

Table XII also includes a comparison with the calculation I of Zofka and Ripka using the density-dependent effective interaction of Negele,[32] and $B1$ interaction of Brink and Boeker.[33]

A glance at Table XII indicates that the calculation of Lee and Cusson (LC), like ours, only semiquantitatively reproduces the total binding energy systematics, the rms radii as well as the energy gaps. For the spherical nuclei, the MY interaction yields deepest and last filled single-particle levels which are more tightly bound though both are overbound with respect to the observed values. For the deformed nuclei the reverse is true and the LC levels are somewhat overbound. The quality of agreement for the energy gaps is about the same and the LC calculation yields radii which are slightly bigger though still small in comparison with the experimental values. In their calculation FBB have not laid emphasis on seeking agreement for the binding energy but rather on the properties which depend mostly on the long-range part of the two-nucleon interaction. Their occupied single-particle energies are not as strongly bound as obtained by LC and in this work. The density-dependent interactions yield results which show an overall better agreement with experiments.

V. CONCLUSIONS

Previous calculations utilizing realistic potentials in calculating effective matrix elements through the unitary-model operator method and subsequently using them in Hartree-Fock type calculations for $2s$-$1d$ shell nuclei, have employed two parameters in their attempts to reproduce the experimental properties of these nuclei: the healing distance of the $^3S_1$ relative state and the choice of the oscillator parameter. The modification of the Yale interaction has essentially removed one of these parametrization procedures since the $^3S_1$ state heals naturally without an additive pseudopotential. The modified Yale potential, which is obtained by decreasing the relative contribution of the tensor component of the two-nucleon potential to the total potential, leads to Hartree-Fock results for the binding energies of nuclei in the $2s$-$1d$ shell, which are better than those of the R and Y interactions by 20–6% when the same prescription, with nearly the same parameters, is used. The modified Yale potential also yields improvement in the calculated deformation parameter β for the nuclei ^{20}Ni, ^{24}Mg, ^{28}Si, and ^{32}S. The improvement amounts to about 12% over the value given by the Y interaction and about 10% for the R interaction.

For the closed-shell nuclei the improvement is significant for the ^{16}O nucleus; the calculated binding energy per nucleon for the MY interaction is −8.14 MeV, as opposed to −9.80 MeV for the Y interaction with a little larger healing distance, and the experimental value is −7.98 MeV. The rms radius is also slightly improved as shown in Table IV. The ^{40}Ca results represent a marked difference to the improving trend which is evidenced in the lighter nuclei; the binding energy of −12.94 MeV is to be compared with the value −11.23 MeV for the R interaction but with a much greater healing distance for the $^3S_1$ relative state. Both the interactions give considerable overbinding since the experimental value is −8.55 MeV per nucleon.

The most striking difference, however, is evidenced in the HF results for ^{40}Ca as obtained with the MY and Y interaction using effective matrix elements calculated with the same values for the oscillator parameter, the $^3S_1$ state healing distance, and the level shift parameter Δ; the binding of −12.93 MeV per nucleon is to be compared with that of −20.06 MeV per nucleon. Evidently the reduction of the tensor component of the two-nucleon potential is responsible for this large reduction in binding energy.

It is thus safe to conclude that a reduction of the strength of the tensor component of the two-nucleon Yale potential without affecting the other quantities calculable from the potential leads to some improvement in the nuclear structure properties of the $2s$-$1d$ shell nuclei. However, the method still leads to the following general failures: (1) For spherical nuclei, the method gives single-particle energies for the low orbitals that are twice as deep as the observed values while the unoccupied levels are somewhat underbound. (2) It does not seem possible to achieve simultaneously an agreement for the binding energies and the rms radii, though one can obtain improved results by varying the oscillator parameter from nucleus to nucleus and using larger expansion bases as well as varying the strength of the level-shift parameter Δ. Further improvements in the results can be obtained by pursuing the generalized Hartree-Fock-Bogoliubov approach.[34,35]

ACKNOWLEDGMENTS

The authors are grateful to Professor G. Breit for providing them with the modified version of the Yale potential without which this work could not have been possible. It is also desired to thank Professor M. H. Hull, Jr., and Dr. R. Nisley for supplying the machine programs needed in this calculation. The practical assistance of Dr. Nisley is also gratefully acknowledged.

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