Further Investigation of Two-Body Interactions in Hartree-Fock Calculations*

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Hartree-Fock calculations with two-body forces are presented in several nuclei, taken as spherical, from He^4 to Pb^{208}. We first present the results obtained with the best (SP1 and SP2) of the recent smooth semirealistic interactions of Saunier and Pearson. These yield good binding energies and radii except in the vicinity of Ni^{56}. However, the spectra in nuclei with spin-unsaturated shells are poor: The spin-orbit splittings in such nuclei are very small (if not negative), and, in particluar, in Pb^{208} the level ordering near the top of the Fermi sea is incorrect. This feature does not allow meaningful extrapolation to the superheavy region with these potentials.

In an attempt to find a two-body interaction allowing such an extrapolation, we modify SP1 and find that with a very strong positive triplet-even phenomenological tensor force the Pb^{208} spectrum is very much improved, and the level ordering and density of uppermost occupied states are comparable to the experimental ones. As a result, Pb^{208} is now found doubly magic, together with a good binding energy and radius. The magic nature of O^{16}, Ca^{40}, Ca^{48}, Ni^{56}, and Zr^{90} is also reproduced by the modified SP1. Consequently this interaction provides new possibilities for valuable extrapolation to the superheavy region with a two-body force.

1. INTRODUCTION

The underlying aim in nuclear Hartree-Fock (HF) calculations is to reproduce self-consistently from an assumed basic interaction (be it realistic or effective, phenomenological or not) the properties of known nuclei, such as energies and radii, spectra, magic numbers, etc. If and when known nuclei can be understood (to some reasonable accuracy) in this self-consistent manner, one can then attempt to extrapolate to less well-known regions of the Periodic Table, such as neutron-rich or superheavy nuclei.

Ideally one should use in these calculations a G-matrix effective interaction rigorously derived from the real nucleon-nucleon (N-N) interaction. However, despite the great vigor with which this approach has been followed, notably at Oak Ridge and Carnegie-Mellon University, the most recent calculation[1] on doubly-closed-shell nuclei shows a less than complete agreement with experiment. Actually this disaccord is hardly surprising, in view of the fact that only two-body clusters are taken into account in this calculation, while it is known that with the N-N potential used, that of Reid,[2] one must take into account higher-order clusters[3] and the meson-theoretic three-body force[4] before acceptable results for nuclear matter are obtained.

Accordingly, in the interest of simplicity and precision, many workers have preferred to sacrifice some rigor and introduce a phenomenological element. Particularly noteworthy are the density-dependent effective interactions of Nemeth and Vautherin[5] and of Negele,[6] derived from the Reid force to yield the same matrix elements in nuclear matter as the G matrix, and designed to be used in the local-density approximation. However, the short-range part of the effective interaction is then renormalized to give the correct properties of nuclear matter, thereby presumably simulating the needed higher-order effects.

In the class of interactions which lean entirely on phenomenology is the Skyrme-type potential of Vautherin and Brink (VB),[7] which incorporates a three-body zero-range force to simulate the density dependence of the effective interaction. HF calculations with this potential[7] have yielded very good results all along the stability line. While this phenomenological approach does not enhance our understanding of nuclear structure to the same degree as if the same results were obtained through the more rigorous program typified by Ref. 1, we believe the importance of the phenomenological approach lies in the possibility it offers of using the HF method to extrapolate to neutron-rich or superheavy nuclei. Calculations with the VB interaction in the superheavy region[8] predict $Z = 114$ to be a magic nucleus. This is in accord with phenomenological single-particle calculations of Nilsson[9] and Meldner.[10]

On the other hand, this result is in conflict with

the first-order HF calculations of Bassichis and Kerman,[11] who, working with the Tabakin potential,[12] find $Z = 120$ to be the magic proton number in this region. Although in first order the Tabakin potential grossly underbinds nuclei and gives very small radii, Bassichis and Kerman find the magic numbers up to Pb^{208}, and thus the prediction in the superheavy region must not be regarded as being completely unreliable. However, it must be kept in mind that the single-particle spectrum is quite sensitive to the radius.

We note that taking account of the second- and third-order perturbation corrections[13] using the Tabakin potential leads to much better binding energies. However, the inclusion of these corrections would be prohibitively time consuming in heavy and superheavy nuclei. It would clearly be desirable therefore to perform HF calculations with other interactions which work well in first order in known nuclei, but which have nevertheless a closer relation to the real N-N force than the VB interaction.

As for the Negele and Nemeth-Vautherin interactions, to our knowledge no search of the superheavy magic numbers has been performed with these. In any case, for heavy nuclei a one-body spin-orbit component, not derived in a completely self-consistent manner from the basic force, is introduced. A similar remark applies to some other calculations,[14,15] where the lack of vector and tensor components in the basic two-body interaction used has led to the introduction of a phenomenological one-body spin-orbit term. In both these cases the microscopic origin of the nuclear spin-orbit splitting is not clearly ascertained. We are informed that D. W. L. Sprung and X. Campi-Benet are extracting from the Reid force a full effective interaction containing both vector and tensor components, and one awaits with interest the outcome of this ambitious program.

On the other hand, regarding first-order HF calculations with two-body interactions, it was noted several years ago (see Svenne's Ph. D. thesis[16] and Kerman's Cargèse lectures[13]) that the lack of density dependence does not allow a simultaneous fit to the total binding energy, the nuclear radius, and all the single-particle energies (cf. Refs. 15–18). This can be clearly understood from the following relation which holds in first-order HF theory with a two-body density-independent force:

$$E = \tfrac{1}{2} \sum_{\lambda\,\mathrm{occ}} (t_\lambda + e_\lambda), \tag{1}$$

which does not appear to be satisfied experimentally in the (light) nuclei where all the e_λ's can be measured. Density-dependent or three-body forces will introduce an additional rearrangement-energy term which could remove the discrepancy.

Nevertheless, since the above relation constrains only the sum of single-particle energies, there remains the question as to whether a two-body interaction can give an exact radius, a good binding energy, and a reasonable spectrum near the top of the Fermi sea, that is, at least the correct sequence of single-particle levels (if not the absolute values of the energies), with large gaps at the known magic numbers. If these characteristics are reproduced, we then have the possibility of a valuable extrapolation to the superheavy region. None of the various purely two-body interactions which have been used so far in HF calculations[15–18] was able to satisfy all these conditions.

In order to test whether the recently developed semirealistic effective interactions of Saunier and Pearson[19] (SP) [in which the main new feature is the conformity to the one-boson-exchange-potential (OBEP) tail] could lead to better results, first-order HF calculations were performed in several nuclei along the stability line. Note that it would be meaningless to introduce second- and higher-order perturbation corrections, as the interactions are effective. We present here the results obtained with the best potentials of Ref. 19, SP1 and SP2, for He^4, O^{16}, Ca^{40}, Ca^{48}, Ni^{56}, Zr^{90}, Sn^{120}, and Pb^{208}. For all these nuclei, the simplest nuclear configuration, that of spherical symmetry, is assumed. The Coulomb interaction was added to, and the center-of-mass energy operator was subtracted from, the nuclear Hamiltonian before diagonalization. Extensive results in deformed nuclei with $A \leq 41$ can be found in the study made by Cusson and Lee[20] with SP2.

It will be seen that although they yield better energies and radii than other two-body forces in first order, the interactions SP1 and SP2 give very poor single-particle spectra in spin-unsaturated-shell nuclei and, in particular, fail to predict Pb^{208} as a magic nucleus. Attempts were made to rectify this defect by modifying in turn the various components of SP1. We will show that, through a drastic increase of the phenomenological triplet-even tensor component, an interaction (SP1 mod) is obtained which improves considerably the spectra of nuclei with neutron and proton spin-unsaturated shells, such as Ni^{56} and Pb^{208}.

With this modified SP1 interaction, Pb^{208} will indeed be found doubly magic, exhibiting the correct sequence of levels near the top of the Fermi sea, with a very good radius and a good binding energy.

2. PROCEDURE

For an A-particle system, we define the HF wave function as the Slater determinant Ψ_{HF} which mini-

mizes the quantity

$$E_{\mathrm{HF}}=\left\langle \Psi_{\mathrm{HF}}\left| H-\frac{P^2}{2mA}\right|\Psi_{\mathrm{HF}}\right\rangle . \tag{2}$$

Since in this calculation spherical symmetry is assumed for the nuclei studied, the single-particle states ψ_α composing Ψ_{HF} have good quantum numbers l, j, m. τ distinguishes between protons and neutrons. Each ψ_α is projected on a truncated harmonic-oscillator basis of the parameter γ $(=\hbar/m\omega)$ according to the expansion

$$\psi_\alpha=\xi_\tau^{1/2}\mathcal{Y}_{l\frac{1}{2}j}^{m}(\hat{r})\sum_{n=0}^{d_\alpha-1}C_n^\alpha R_{nl}(r^2/\gamma), \tag{3}$$

with n the principal radial quantum number and $R_{nl}(x)$ defined as in the work of Brody and Moshinsky.[21] The dimensionality d_α has been taken equal to 4 for all α, unless otherwise indicated. We have made a study of the adequacy of this choice of dimensionality elsewhere.[22] The expansion coefficients C_n^α are determined by solving the self-consistent HF equations via an iterative procedure.

It is known that when the center-of-mass energy operator is subtracted as in Eq. (2), the one-body kinetic energy operators drop out of the HF Hamiltonian, and the eigenvalues of the self-consistent field are

$$e_\alpha=\sum_{\beta=1}^{A}\left\langle \alpha\beta\left| V_{12}+\frac{2p_{12}^{\,2}}{mA}\right|\alpha\beta\right\rangle . \tag{4}$$

V_{12} is the two-body force and $\vec{\mathrm{p}}_{12}$ is the relative momentum operator.

The definition of "single-particle" energies (which we denote by ϵ_λ) and their comparison with the experimental one-particle-removal energies are discussed at length by Bassichis and Strayer[23] and by Köhler and Lin.[24] We here assume

$$\epsilon_\lambda=E_{\mathrm{HF}}(A)-\tilde{E}_{\mathrm{HF}}^{\lambda}(A-1), \tag{5}$$

where the single-particle wave functions are taken to be identical in the nuclei A and $A-1$, that is, the orbital-rearrangement correction is neglected (this is denoted by the symbol $\tilde{}$). This approximation seems to be acceptable, at least near the top of the Fermi sea, as some results of Refs. 23, 24 and of Faessler and Wolter[25] seem to suggest.

Since we have removed the center-of-mass energy from the Hamiltonian in Eq. (2), the relation between the single-particle energies ϵ_λ and the eigenvalues ϵ_λ of the self-consistent field becomes, through Eq. (5), for occupied and unoccupied states, respectively.

$$\epsilon_{\lambda\,\mathrm{occ}}=\frac{Ae_\lambda-\chi_\lambda+t_\lambda+E_{\mathrm{c.m.}}-T}{A-1} \tag{6a}$$

and

$$\epsilon_{\lambda\,\mathrm{unocc}}=\frac{Ae_\lambda+\chi_\lambda-t_\lambda+E_{\mathrm{c.m.}}-T}{A+1}, \tag{6b}$$

where

$$T=\sum_{\alpha=1}^{A}t_\alpha, \tag{7}$$

$$E_{\mathrm{c.m.}}=\left\langle \Psi_{\mathrm{HF}}\left|\frac{P^2}{2mA}\right|\Psi_{\mathrm{HF}}\right\rangle=T-\sum_{\alpha\beta=1}^{A}\left\langle \alpha\beta\left|\frac{p_{12}^{\,2}}{mA}\right|\alpha\beta\right\rangle_{\mathrm{AS}}, \tag{8}$$

$$\chi_\lambda=t_\lambda+\sum_{\beta=1}^{A}\langle\lambda\beta|V_{12}|\lambda\beta\rangle_{\mathrm{AS}} . \tag{9}$$

The charge radius calculated is the rms value of the proton distribution with the proton radius $a_p=0.8$ fm[26] folded in:

$$r_C=\left[\frac{1}{A}\sum_{\alpha=1}^{A}\langle\psi_\alpha|r^2(\tfrac{1}{2}+\tau)|\psi_\alpha\rangle+a_p^{\,2}\right]^{1/2} . \tag{10}$$

To compute the numerous matrix elements of two-body operators needed in the HF treatment of heavy and superheavy nuclei, we have developed a fast numerical method, based on the following expansion:

$$\langle\alpha,\beta;JT|O|\gamma,\delta;JT\rangle=\sum_{nn'l'}Q^{\alpha\beta\gamma\delta JT}_{Sqnn'l'}\langle nl\|O^q_{ST}(r,p)\|n'l'\rangle , \tag{11}$$

where $q=0, 1, 2$ serves to distinguish the various tensorial orders of O: and the other labels represent the usual quantum numbers. The geometrical coefficients Q do not depend on the operator O. Therefore they have been calculated once and for all and stored on magnetic tapes. Note that if we consider only spherical nuclei, the set of coefficients Q can be reduced by performing a sum on the total angular momentum J. In the sum (11), we limit ourselves to relative $l, l'\leq 5$ for the nuclear potential, but for the Coulomb force and relative momentum operator p^2, we include all l's permitted by the conservation laws.

Regarding calculations in nuclei with incomplete j shells (for example when studying the effect of removing some pairs of nucleons from the uppermost shell), we adopt the procedure of Bassichis and Kerman,[11] that is, we consider the nuclei as spherical, but with an occupation parameter θ_j in each incomplete shell, defined by

$$\theta_j=N_j/(2j+1), \tag{12}$$

where N_j is the population of the shell j. In order to avoid difficulties due to time reversal, we limit ourselves to even N_j.

3. INTERACTIONS

The first two potentials considered in this work, SP1 and SP2, are among the four semirealistic quadratically velocity-dependent effective interactions developed by SP.[19] They are of the form

$$V^{\text{eff}} = V^{\text{OBEP}} + V^{\text{phen}}, \tag{13}$$

where V^{OBEP} is the tail of the Bryan and Scott potential,[27] cut off at 1 fm in all terms except the even-state tensor force, cut off at 2 fm. The short-ranged phenomenological part is of the form

$$V^{\text{phen}} = \frac{\hbar^2}{m}\left[A_c e^{-\alpha_c^2 r^2} + \frac{B}{\hbar^2}(p^2 e^{-\beta^2 r^2} + e^{-\beta^2 r^2} p^2) + A_v r^{\gamma_v} e^{-\alpha_v^2 r^2} \vec{L}\cdot\vec{S} + A_t r^{\gamma_t} e^{-\alpha_t^2 r^2} S_{12}\right]. \tag{14}$$

The parameters of the short-ranged part were adjusted[19] to make SP1 and SP2 both realistic in the odd nucleon-nucleon states, and each realistic in one of the even states. SP1 satisfies the scattering N-N data in the singlet-even, but not the triplet-even state, and vice versa for SP2. The departure from a completely realistic interaction was designed in both cases to saturate nuclear matter in first order at $E/A = 16$ MeV, $k_F = 1.35$ fm^{-1}. Results of calculations with SP3 and SP4 (to be found in Ref. 22) are not presented here, since radii obtained with SP3 are much too small (as found with other realistic potentials[16]), and since the results with SP4 are quantitatively poorer than those with SP1 and SP2. We later present a third interaction, called SP1 modified, which differs from SP1 only in the strength of the triplet-even phenomenological tensor component, and is thus still realistic in three spin-isospin states.

Note that although the interactions considered in this work are semirealistic, they are in fact effective and therefore should be used in first-order calculations only.

4. RESULTS

The effect on the total binding energy of the truncation of the harmonic-oscillator basis has been studied several times, and it is known that a small dimensionality is quite adequate for light and medium nuclei[16-18,22]; in other words even with a small basis, E_{HF} does not depend strongly on the harmonic-oscillator parameter $\gamma = \hbar/m\omega$ for these nuclei. In heavy (e.g., Pb^{208}) and superheavy nuclei, the effects of truncating the basis are more critical. For this reason, we use a dimensionality d = constant = 4, which permits the use of the same value of γ for a wide range of nuclei. From Fig. 1 it is clear that taking $\gamma = 2.5$ in very light nuclei (He^4, O^{16}), $\gamma = 4.0$ in medium nuclei (Ca^{40}, Ca^{48}, Ni^{56}, Zr^{90}, Sn^{120}), and $\gamma = 5.5$ in heavy nuclei (Pb^{208}) are reasonable choices. One may feel uneasy about the fact that the $s_{1/2}$ states in Pb^{208} have only one degree of freedom. However, we have verified that the change in E_{HF} when d = constant = 3 (then the $s_{1/2}$ states have no degree of freedom) instead of $d = 4$ is only 0.15 MeV per particle, and that the ordering of single-particle levels (which is of great importance when looking for a possible shell closure) is not modified.

Tables I and II give a comparison of our results of binding energy per particle and charge radius for the two interactions SP1 and SP2 to experiment and to the results of first-order HF calculations of some other groups. The entry SP1 mod will be discussed later. Only first-order results are reported, because our aim is to search for an interaction which would provide a valuable tool for extrapolation to the superheavy region in first order, and which must therefore perform well in known nuclei to the same order.

It is seen that SP2 fits (to within 0.8 MeV per particle) the experimental binding energies from He^4 to Pb^{208} well, except around Ni^{56}. The radii are slightly too small except for He^4, but the percentage error always remains below 7%. In contrast, SP1 fits the charge radii above He^4 well, but with a slight underbinding of about 2 MeV per particle. Neither potential explains the experimental observation that $r_c(Ca^{40}) > r_c(Ca^{48})$.

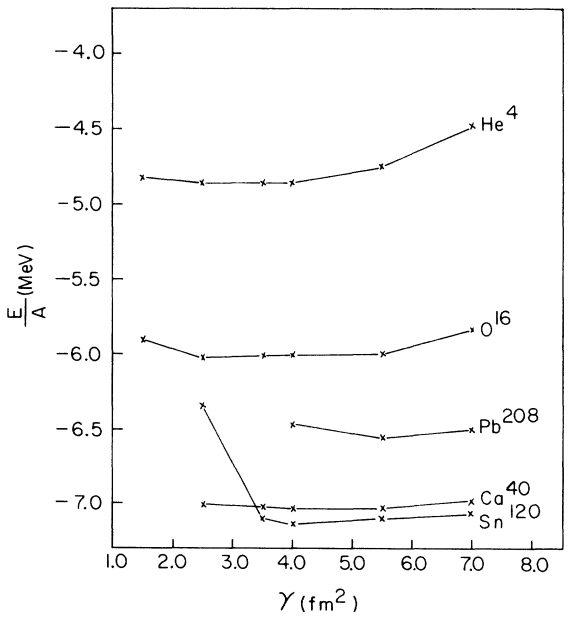

FIG. 1. Binding energies per particle obtained with SP1 for several nuclei versus oscillator parameter γ (fm^2), using a constant dimensionality equal to 4 for every single-particle level.

TABLE I. Binding energies per particle (MeV) given by the potentials SP1, SP2, and SP1 mod, compared with experiment [J. H. E. Mattauch *et al.*, Nucl. Phys. 67, 1 (1965)] and with the first-order results obtained by Kerman, Svenne, Villars, and Bassichis (KSVB) (Refs. 13, 16); Tarbutton and Davis (TD) (Ref. 18); Pirès, De Tourreil, Vautherin, and Vénéroni (PDVV) (Ref. 15); Vatherin and Brink (VB) (Ref. 7); and Negele (Ref. 6).

$\gamma=\frac{\hbar}{m\omega}$ (fm^2) \ Nucleus	He^4	O^{16}	Ca^{40}	Ca^{48}	Ni^{56}	Zr^{90}	Sn^{120}	Pb^{208}
	2.5	2.5	4.0	4.0	4.0	4.0	4.0	5.5
Pot SP1	−4.86	−6.02	−7.04	−6.72	−6.16	−7.16	−7.14	−6.55
Pot SP2	−7.04	−7.92	−8.47	−7.93	−7.12	−8.11	−7.93	−7.00
SP1 Mod	−4.86	−6.02	−7.04	−6.75	−7.25	−7.14	−7.13	−6.90
KSVB	−0.03	−2.41	−3.65	−3.45		−3.98		−2.00
TD		−4.81	−5.64	−5.50	−4.97	−5.99		−5.49
PDVV		−6.06	−6.40	−5.70				−5.40
VB		−8.22	−8.64	−8.93		−8.81		−7.89
Negele		−6.75	−7.49	−7.48		−7.85		−7.53
Expt	−7.08	−7.98	−8.55	−8.67	−8.64	−8.71	−8.51	−7.87

As an aside, we note that the charge radius of He^4 should be treated in a special manner: because of the importance of center-of-mass motion in this very light nucleus, the charge radius should be calculated through

$$r_c^2=\frac{1}{A}\langle\Psi_{\rm HF}|\sum_{i=1}^{A}(\vec{r}_i-\vec{R})^2(\tfrac{1}{2}+\tau)|\Psi_{\rm HF}\rangle+a_p^2\,, \qquad (15)$$

where

$$\vec{R}=\frac{1}{A}\sum_{i=1}^{A}\vec{r}_i\,, \qquad (16)$$

instead of through Eq. (10), which we have used. With Eq. (15) smaller He^4 radii, in better accord with experiment, would be found, e.g., 1.65 fm for SP2, as communicated to us by Cusson and Lee.[20]

On the whole, the binding energies and nuclear radii given by SP1 and SP2 (each of which is realistic in three out of four spin-isospin states) are better than those obtained, to our knowledge, with any other realistic or semirealistic two-body interaction in the literature. Comparison in Tables I and II with the first-order results of Kerman *et al.* (KSVB),[13,16] Tarbutton and Davies (TD),[18] and Pirès *et al.* (PDVV)[15] shows that the binding energies given by SP1 and SP2 are generally closer to experiment. As for the radii, those obtained with SP1 are on the whole better than those of the above groups, whereas SP2 leads to smaller radii than those of PDVV.

It is to be noted that with second- and third-order perturbation corrections[13] the Tabakin potential gives a nuclear binding energy quite close to the experimental value. However, the radius apparently remains very small, a fact which can affect strongly the single-particle spectrum and the Coulomb energy.

In the case of Brueckner-Hartree-Fock calcula-

TABLE II. Nuclear charge radii (fm) given by the potentials SP1, SP2, and SP1 mod, compared with experiment [Ref. 26 and R. Hofstadter and H. R. Collard, *Nuclear Radii, Landolt Börnstein* (Springer, Berlin, 1967); J. B. Bellicard and K. J. Van Oostrum, Phys. Rev. Letters 19, 242 (1967)] and other results as in Table I.

$\gamma=\frac{\hbar}{m\omega}$ (fm^2) \ Nucleus	He^4	O^{16}	Ca^{40}	Ca^{48}	Ni^{56}	Zr^{90}	Sn^{120}	Pb^{208}
	2.5	2.5	4.0	4.0	4.0	4.0	4.0	5.5
Pot SP1	2.12	2.79	3.47	3.55	3.87	4.28	4.64	5.51
Pot SP2	1.86	2.54	3.28	3.34	3.73	4.10	4.45	5.25
SP1 mod	2.12	2.81	3.51	3.57	3.79	4.33	4.69	5.46
KSVB (mass radius)	1.98	2.39	2.84	2.93		3.36		
TD		2.67	3.30	3.34	3.61	4.03		5.14
PDVV		2.68	3.40	3.44				5.49
VB		2.68	3.41	3.46		4.22		5.44
Negele (point proton)		2.71	3.41	3.45		4.18		5.37
Expt	1.67	2.73	3.50	3.49	3.84	4.30		5.52

TABLE III. The proton single-particle energies ϵ given by SP1 and SP2, together with some experimental values. The calculated average binding energy of the protons is also given. Unoccupied levels are underlined.

	O^{16} $\gamma=2.5$ fm^2			Ca^{40} $\gamma=4.0$ fm^2			Ca^{48} $\gamma=4.0$ fm^2			Ni^{56} $\gamma=4.0$ fm^2		
	SP1	SP2	Exp	SP1	SP2	Exp	SP1	SP2	Exp	SP1	SP2	Exp
$1s_{1/2}$	−45.0	−58.7	−44.	−67.0	−78.1	−77.	−71.3	−78.5		−69.5	−75.6	−57.
$1p_{3/2}$	−17.7	−22.9	−19.	−39.9	−46.7	−32.	−46.4	−51.0		−46.0	−50.4	−42.
$1p_{1/2}$	−14.3	−17.5	−12.	−37.6	−43.8		−45.1	−51.0		−46.4	−54.0	−37.
$1d_{5/2}$	2.6	2.7	−1.	−16.2	−19.1	−16.	−22.8	−24.7		−22.9	−24.9	−23.
$1d_{3/2}$	5.9	7.3		−12.4	−14.2	−8.	−20.9	−24.4	−17.	−23.2	−29.2	−13.
$2s_{1/2}$	3.1	2.6		−12.4	−13.8	−12.	−17.9	−18.9		−17.6	−18.6	−10.
$1f_{7/2}$				2.5	2.6		−3.0	−2.5	−10.	−3.2	−2.9	−7.
$1f_{5/2}$				6.2	7.2		−0.5	−1.3	−6.	−2.1	−5.6	
$2p_{3/2}$				3.5	5.8	0.7	−0.4	0.4	−7.	0.3	0.9	
$2p_{1/2}$				4.4	7.5		0.5	0.7	−4.	0.8	0.1	
E_p/Z	−5.2	−7.0		−5.4	−6.6		−8.5	−9.4		−4.0	−4.8	

tions (e.g., see Ref. 1), the binding energy obtained is too small, of the order of 2 MeV per particle, whereas the radius is fairly good.

While it is not clear exactly which features of SP1 and SP2 allow generally better results than the forces used by the above groups, we note that inclusion of the OBEP tail (which, according to the Moszkowski-Scott analysis, should be present at long range in the effective interaction) has given additional freedom in the determination of the phenomenological term in the potentials, since this term need then simulate only the short-range part of the effective interaction instead of its entirety.

We call attention to the very good results obtained by Vautherin and Brink[7] and Negele,[6] also shown in Tables I and II. The decisive factor in these more sophisticated calculations seems to be the density dependence (or the three-body force designed to similate it), which introduces a rearrangement energy, as discussed in the Introduction.

Tables III and IV show the values of ϵ obtained for protons with SP1 and SP2, together with some experimental values.

The spin-orbit splittings $\Delta_l = \epsilon(j_- = l - \frac{1}{2}) - \epsilon(j_+ = l + \frac{1}{2})$ given by SP2 in light nuclei (O^{16} and Ca^{40}) are fairly good. Those yielded by SP1 are smaller (about half the experimental values). This is somewhat surprising, as these two poten-

TABLE IV. Continuation of Table III.

	Zr^{90} $\gamma=4.0$ fm^2			Sn^{120} $\gamma=4.0$ fm^2			Pb^{208} $\gamma=5.5$ fm^2		
	SP1	SP2	Exp	SP1	SP2	Exp	SP1	SP2	Exp
$1s_{1/2}$	−79.1	−84.0		−84.0	−85.7		−83.5	−80.6	
$1p_{3/2}$	−58.6	−62.9		−64.7	−67.4		−69.4	−67.9	
$1p_{1/2}$	−57.6	−63.0		−64.6	−68.3		−69.4	−68.9	
$1d_{5/2}$	−37.5	−40.5		−44.8	−47.2		−53.9	−53.1	
$1d_{3/2}$	−35.9	−40.5		−44.3	−48.0		−53.9	−55.0	
$2s_{1/2}$	−31.7	−33.1		−39.7	−39.7		−49.1	−48.0	
$1f_{7/2}$	−17.4	−18.7		−25.4	−26.8		−37.7	−37.3	
$1f_{5/2}$	−15.1	−18.1		−24.1	−27.0		−37.5	−39.7	
$2p_{3/2}$	−11.2	−10.9	−8	−19.2	−18.6		−30.7	−29.7	
$2p_{1/2}$	−10.1	−10.5		−18.6	−18.5		−30.4	−30.2	
$1g_{9/2}$	0.4	0.8	−5	−7.6	−7.8		−21.5	−21.1	
$1g_{7/2}$	3.3	2.3		−5.2	−6.8		−21.0	−23.7	−11.5
$2d_{5/2}$				−1.9	−1.0		−13.7	−12.7	−9.8
$2d_{3/2}$				−0.9	−0.8		−13.0	−13.3	−8.5
$3s_{1/2}$				0.8	1.4		−10.8	−9.2	−8.0
$1h_{11/2}$							−6.0	−5.5	−9.4
$1h_{9/2}$							−4.7	−7.5	
E_p/Z	−6.5	−7.1		−7.1	−7.4		−6.1	−5.9	

tials have the same triplet-odd vector force, but may perhaps be understood partly as an effect of the difference in radii given by SP1 and SP2. From previous constrained HF calculations,[28] where the radius was constrained to various values, it was verified that (for a given potential) the splitting increased as the radius decreased.

As for nuclei with spin-unsaturated shells (in which only one of the subshells j_+, j_- is filled), the Δ_l calculated with SP1 for the deeper levels are completely destroyed; with SP2 they are even negative. Such a result has already been found.[18,29] This part of the spectrum is, however, not known experimentally. More alarming is the fact that with SP2 this situation prevails also for the upper part of the spectrum. In Ni^{56} and Pb^{208} the first "unoccupied" levels lie even below the last "occupied" levels, that is, the order in which the levels have been filled seems to be incorrect. But if we switch the filling order (e.g., calculate Hg^{206} with the $1h_{9/2}$ proton level filled, leaving $1h_{11/2}$ empty), the first unoccupied level (in the example, $1h_{11/2}$) is again found below the last occupied level ($1h_{9/2}$). This difficulty is a defect of the interaction, since it does not occur with SP1. For the latter, the splittings near the top of the Fermi sea are always positive, but nevertheless too small, especially for the spin-unsaturated shells. For instance, the proton $1h_{11/2}$ level of Pb^{208} lies above $3s_{1/2}$, whereas it should be between the $2d$ levels. With such very small spin-orbit splittings it is impossible to predict the correct magic numbers.

We have examined the total-energy curve vs Z for SP1 in the lead region,[22] not shown here. A large break in slope, a characteristic of a magic number,[11] appears at $Z=70$, but not at $Z=82$, favoring $Z=70$ as the magic nucleus in this region. This is confirmed by the large energy gap (7.5 MeV) between highest occupied and lowest unoccupied levels for $Z=70$. For $Z=82$ this gap is much smaller (1.3 MeV).

This shows that SP1, together with SP2 (whose results are very similar), are inadequate for heavy nuclei, since they cannot predict Pb^{208} as being magic.

The lack of spin-orbit splitting also explains, at least partly, the serious underbinding around Ni^{56}, as long as we stay in the context of a spherical HF basis. This lack of splitting results in very underbound $f_{7/2}$ subshells, which in the configuration we have used contain 16 of the Ni^{56} nucleons. Some HF calculations[29] have shown that by deforming the HF basis, one may with some potentials obtain much more binding for Ni^{56}. We have not attempted any calculations in a deformed basis.

Since the poor spectra found with the SP potentials in spin-unsaturated-shell nuclei do not allow meaningful extrapolation to the superheavy region, numerous attempts to improve these spectra, while remaining with the simpler two-body forces, were made. Extensive studies of modifications to the various parts of the interaction, usually employing SP1 as starting point, were carried out. Modifications in the two-body vector component of the force and in the scalar component (notably its relative weight in the various spin-isospin states) were attempted, but did not lead to sensible general improvements for all nuclei.

It was noticed however that a drastic increase in the tensor force has a considerable effect on the spectra of spin-unsaturated-shell nuclei. We here present a potential (SP1 mod) differing from SP1 in the triplet-even phenomenological tensor part. The latter has been changed in sign and multiplied by a factor of 18, slightly smaller than that used in a previous report.[22] This represents a large increase; the tensor matrix elements $\langle nl|S_{12}V_T(r)|n'l'\rangle$ are now -8 to -10 times the corresponding ones of the OBEP tensor cut off at 0.67 fm for $l=0$, $l'=2$, $\gamma=5.5$ fm^2.

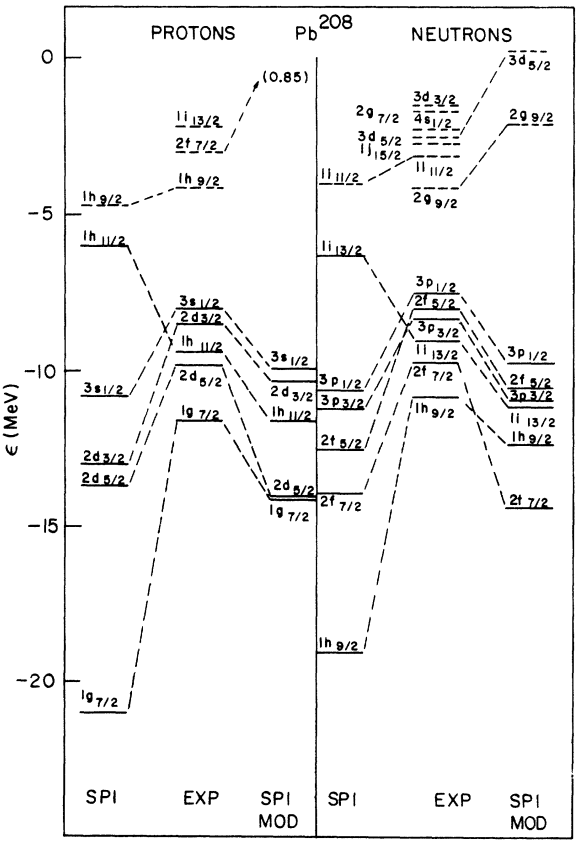

FIG. 2. The uppermost part of the Pb^{208} proton and neutron spectra. Unoccupied levels are indicated by dashed lines.

With this increased tensor force, the Pb^{208} spectrum is very much improved, as shown in Fig. 2. The spin-orbit splittings are greatly increased, and the sequence of occupied levels is now almost perfect. Of utmost importance is the fact that the $1h_{11/2}$ proton level has come down between the $2d$ levels, as in the experimental spectrum. Similarly, the $1i_{13/2}$ level is now between the $2f$ levels.

The entire uppermost part of the spectrum is shifted down with respect to experiment. This may be related to the constraint imposed by Eq. (1) for pure two-body forces, since the total energy and radius are good. The level density of occupied states near the top of the Fermi sea is now very good, and now the Fermi levels for protons and neutrons are almost at the same height, as in the experimental spectrum.

The great increase in the splittings and the fact that the proton $1h_{11/2}$ and neutron $1i_{13/2}$ levels fall to the lower shells now allow the doubly magic nature of Pb^{208} to emerge. This is verified in Fig. 3, where the total energy is plotted vs A, when Z and N are in turn kept constant. The large breaks in slope are seen to occur at $A=208$, $Z=82$, and $N=126$.

Figure 4 shows a less detailed study of some lighter nuclei with spin-unsaturated shells. The total energy E is plotted vs Z, while A is kept constant at 48, 56, and 90. The corresponding values of Z_0 where the energy is a minimum indicate that SP1 mod reproduces the magic nature of Ca^{48}, Ni^{56}, and Zr^{90}. Similar curves could be shown for O^{16} and Ca^{40}. In the case of $A=48$, the minimum at $Z=20$ (Ca^{48}) is not very sharp, a fact related to a small gap in the proton spectrum, as discussed below.

The binding energies given by SP1 mod for the nuclei studied are given in Table I. For O^{16} and Ca^{40} the binding energy remains identical to that given by SP1; this is not surprising, since it is well known that the tensor force contributes very little to the total energy of spin-saturated-shell nuclei.

Moreover SP1 mod in the context of HF calculation in a purely spherical basis, has improved considerably the binding energy of Ni^{56}, though not designed expressly for this purpose. Ni^{56} is now indeed more bound (per particle) than Ca^{40}, as found experimentally. In view of the resulting Ni^{56} spectrum (Fig. 5) and the large gap between occupied and unoccupied states, one may suspect that allowing the HF basis to become deformed would not lead to a more stable solution, contrary to the result found by Parikh and Svenne[29] for the Tabakin potential. As for Ca^{48}, the new interaction has led to a poorer gap in the proton spectrum (Fig. 6), the unoccupied $f_{7/2}$ subshell diving down

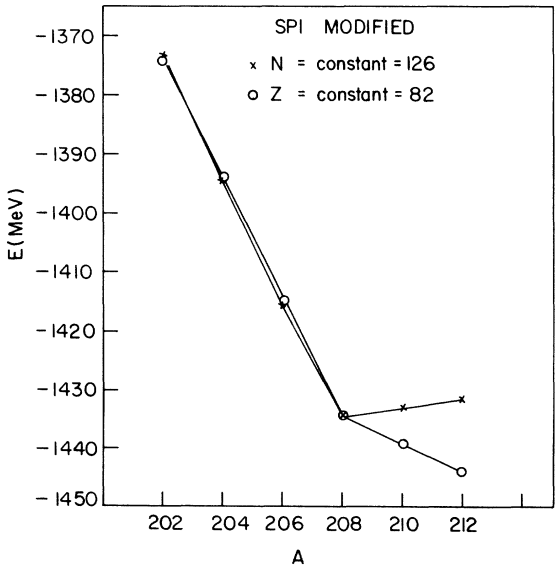

FIG. 3. Total binding energy E vs A when Z or N is kept constant. The calculation is performed with SP1 mod.

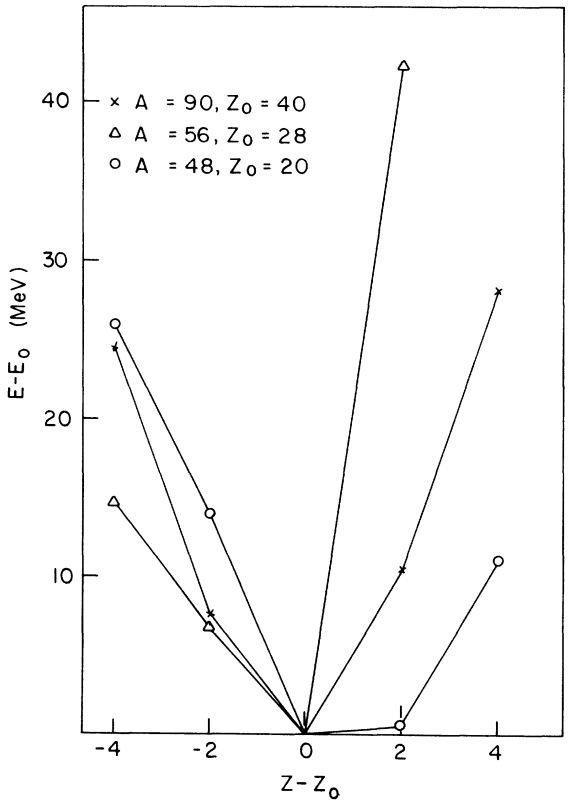

FIG. 4. Total binding energy E vs Z when A is kept constant at 48, 56, and 90, with Z_0 equal, respectively, to 20, 28, and 40. E_0 is in each case the energy of the nucleus $Z=Z_0$, $N=A-Z_0$.

to the occupied levels. Note that the radii of all nuclei are affected very little by the modification of the tensor force (Table II). Since the even tensor force exists only in two-body $T=0$ states, the main effect, to first order, of a change in this force is that an unsaturated neutron (proton) shell affects the proton (neutron) states.

It appears that the modified SP1 interaction yields acceptable results in doubly-closed-shell nuclei, especially those with proton and neutron shells both spin-saturated or both spin-unsaturated. The latter situation prevails in Pb^{208}, and one may suppose, in magic superheavy nuclei (if they exist).

It is possible that the exceptionally strong tensor force could lead to a parity mixing of the single-particle states,[30,31] but in our calculations we have not allowed any such mixing. However, even though our HF solutions might not correspond to the true energy minimum for this interaction, it must be borne in mind that since SP1 mod predicts Pb^{208} as doubly magic in the context of a calculation without parity mixing, and also yields satisfactory results for the lighter doubly-closed-shell nuclei, it should still be suitable for extrapolation to superheavy nuclei, provided the restricted HF treatment is used.

5. CONCLUSIONS

HF calculations with the semirealistic two-body potentials SP1 and SP2, satisfying "known" nuclear-matter properties, and in which the departure from a realistic interaction is concentrated in only one spin-isospin even state, yielded, on the whole, quite good results for the energy per particle and radius of spherical nuclei. In spite of the correct saturation of nuclear matter, the fit was better for light (O^{16} and Ca^{40}) than for heavy nuclei (Pb^{208}); this is associated with the presence of spin-unsaturated shells in real heavy nuclei, whereas spins in nuclear matter are taken as saturated, as in O^{16} and Ca^{40}. Moreover, even medium-mass systems with unsaturated spins, such as Ca^{48} and Ni^{56}, were found to be problematic with these potentials, as had already been discovered by other groups with other two-body forces.

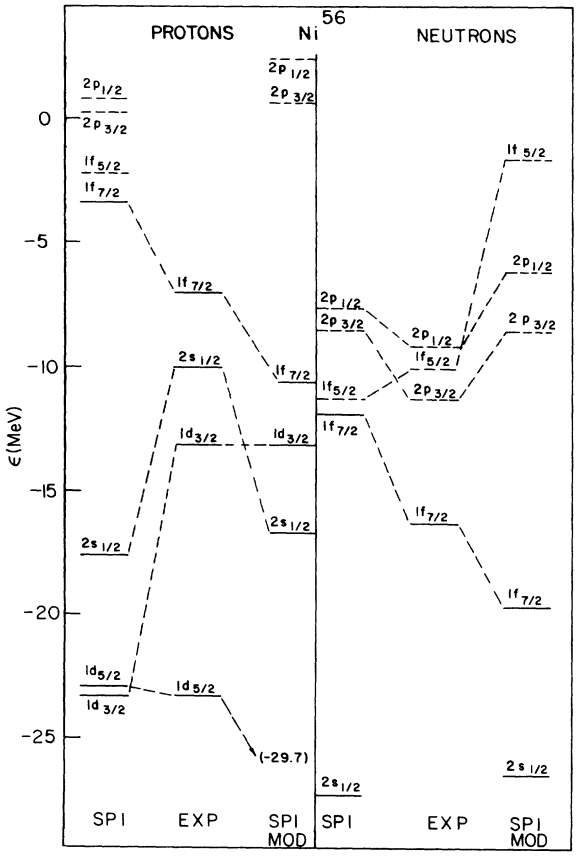

FIG. 5. The upper part of the Ni^{56} proton and neutron spectra. Unoccupied levels are indicated by the dashed lines.

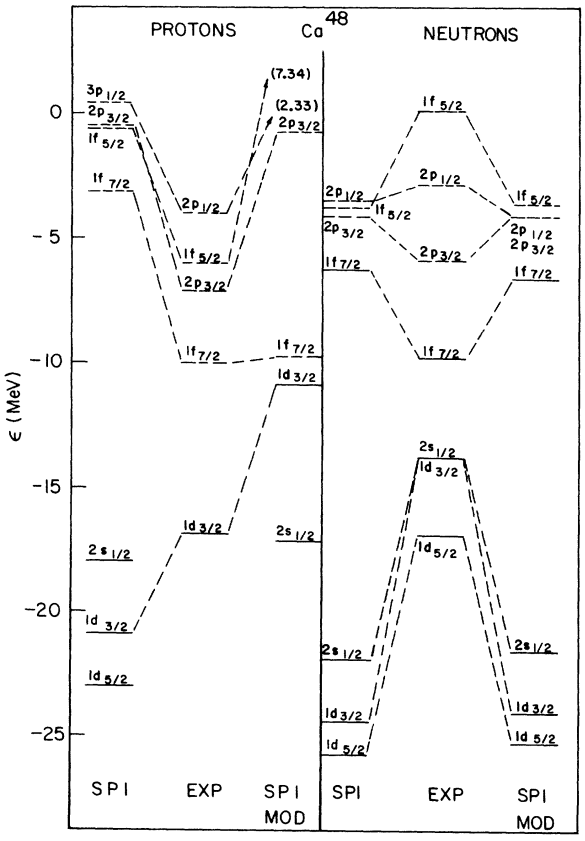

FIG. 6. The upper part of the Ca^{48} proton and neutron spectra. Unoccupied levels are indicated by dashed lines.

Again, while the spectra are acceptable for O^{16} and Ca^{40} (although the splittings are too small), they are poor for Ca^{48}, Ni^{56}, etc. The very small splittings and the underbinding of the unsaturated shells lead to too small a level density near the top of the Fermi sea. Another consequence is that Pb^{208} does not appear as a magic nucleus. By taking a very large positive strength for the phenomenological part of the even tensor force, an effective two-body interaction (SP1 mod) was defined, still realistic in three of the four spin-isospin states and giving a very improved level ordering in the spectrum of Pb^{208}. In particular, for instance, the proton $1h_{11/2}$ state was pushed down between the $2d$ levels, as in the experimental spectrum. With this force then, Pb^{208} is found to be doubly magic, while the binding energy and radius of all the nuclei studied remain quite good, and in some cases even improve (Ni^{56} being the striking case).

This success is accompanied, however, with too large an increase in the spin-orbit splittings of medium spin-unsaturated-shell nuclei. In spite of this circumstance, since the main features of the Pb^{208} spectrum were very well reproduced, it seems possible to make a valuable extrapolation to the superheavy region with this interaction, neglecting parity mixing as discussed in the last section. Such an investigation is currently in progress.

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Role of the Dispersion Effect in the Method of Correlated Basis Functions*

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We develop a consistent procedure for introducing an external single-particle potential into the cluster expansion of the energy expectation value with respect to a correlated wave function. It is shown that the usual Brueckner reaction-matrix approximation may be extracted from the correlated-basis-functions theory by a special treatment of the external potential and an associated special choice of two-body correlation factor.

The problem of uncovering or otherwise imposing a formal connection between the Brueckner-Bethe-Goldstone (BBG) reaction-matrix approach[1] (or other procedures with conventional perturbation theory as a starting point) and the method of correlated basis functions (CBF)[2] has recently absorbed the attention of a number of authors.[3-12] However, we feel that certain misconceptions still persist, especially as regards the presence of a dispersion effect in the variational or Jastrow version of the CBF method, and as regards the introduction of an auxiliary single-particle potential into the associated cluster-expansion scheme. We wish here to clarify the situation by a careful and systematic cluster analysis.

In order to carry through a Jastrow variational calculation as a first step in a more ambitious CBF program, one must know how to calculate expectation values of symmetric sums of one-, two-, ... body operators with respect to a correlated trial state vector, which we write in the form

$$|\Psi\rangle = F|\Phi\rangle, \tag{1}$$

where F is an N-body operator introducing short-range correlations and $|\Phi\rangle$ is a model state vector which would be adequate for describing the state in question in the absence of strong short-range interactions. Very general and powerful – yet intrinsically simple – techniques exist for developing such correlated expectation values in well-defined linked cluster expansions.[13] There is no need to resort to second quantization (in fact this is a disadvantage because of the selective resummations required), or to diagrammatics (except possibly as a visual aid).

There are indeed many kinds of cluster expansions, and only experience can dictate which is best to use for a given physical problem. Four types of expansions were studied by Clark and Westhaus.[13] Among these is the by now familiar Iwamoto-Yamada (IY) expansion,[14] which has been applied to the nuclear-matter problem by Chakkalakal,[15] by Bäckman, Chakkalakal, and Clark,[3] and by Wong,[4] and to O^{16} by Dabrowski.[16] Another procedure studied in Ref. 13, a "factor-cluster" expansion corresponding to the IY expansion, seems preferable on the basis of its formal simplicity and, for finite systems, on the basis of the fact that it is more highly summed than the IY and other familiar expansions.[17] This expansion is sometimes referred to as the Van Kampen expansion,[18] but actually a more specific name is called for; conforming to Ref. 13 we adopt the designation "FIY expansion." The terms of this expansion are arranged according to the number of bodies