Unrestricted Hartree-Fock Treatment of Finite Nuclei*

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A smooth, nonlocal interaction which fits two-body scattering data reasonably well is used in a Hartree-Fock calculation of the binding energies and quadrupole moments of the even-even nuclei with A between 4 and 40. The calculation is unrestricted in that the orbitals of all the particles are determined self-consistently with both radial and angular variations allowed. For the deformed nuclei, a naive rotational correction is made to allow comparison with experiment. The second-order term is computed in a perturbation expansion for which the Hartree-Fock result is the first-order term. The perturbation series apparently converges, and the results to second order agree quite well with experiment. The single-particle energies of the various nuclei are calculated in first and second order with polarization taken into account. Finally, the symmetry energy is studied in the $A=48$ system.

I. INTRODUCTION

SEVERAL two-body interactions[1] have been proposed that fit scattering data with reasonable accuracy and have the advantage of being finite everywhere. Given such a two-body force without the usual hard or infinitely repulsive core, there exists a well-known procedure for obtaining the solution for the many-particle system. The first step in this procedure is a solution of the Hartree-Fock (HF) equations. The application of this method to nuclear structure has become increasingly popular, and complete descriptions of the method have been given by various authors.[2] A brief outline of the general method and the characteristics of the present calculation are given in Sec. II. The Tabakin potential,[3] utilized throughout these calculations, is briefly described there. In Sec. III the results of the HF calculation are compared with experimental binding energies and quadrupole moments.

The perturbation series for which the HF solution serves as the first-order term is described in Sec. IV. An approximate evaluation of the second-order matrix elements[4] was used, and the binding energies calculated to second order are compared with experiment.

In the following section, the meaning of experimental single-particle energies in the HF framework is discussed, and the calculated single-particle energies are presented along with some of the observed values. In Sec. VI, the symmetry energy of the $A=48$ system is considered. Finally, Sec. VII contains general conclusions and an outline of extensions of these calculations presently being performed.

II. THE HARTREE-FOCK PROCEDURE

The Hartree-Fock procedure[2] enables one to find the best determinantal solution of the variational equation

$$\delta(\psi|H|\psi)=0. \tag{1}$$

This leads in a straightforward manner to the equation

$$\langle\alpha|h|\beta\rangle=\langle\alpha|t|\beta\rangle+\sum_{\lambda}\langle\alpha\lambda|V_A|\beta\lambda\rangle=\epsilon_\alpha\delta_{\alpha\beta}, \tag{2}$$

which states that the single-particle orbitals, λ, which enter into the determinantal wave function ψ are those that diagonalize the HF Hamiltonian h. Here t is the kinetic energy; V_A is the antisymmetrized two-body interaction; α and β represent an arbitrary representation; and the summation on λ is restricted to occupied orbitals. The unknown orbitals are expanded in some representation, and the expansion coefficients are found self-consistently via an iteration procedure. The distinguishing characteristics of the various HF calculations[5] being carried out are the choice of H, the truncation of the space, the restriction placed on the expansion of λ, and the nuclei considered.

The force chosen here was the separable, nonlocal force of Tabakin.[3] This force has been used previously in HF calculations with reasonable success.[6] Explicitly, the force is

$$V(\mathbf{r},\mathbf{r}')=\frac{\hbar^2}{\mu}\sum_{JTS}\sum_{Mll'}\{-g_l{}^{JTS}(r)g_{l'}{}^{JTS}(r')+h_l{}^{JTS}(r)h_{l'}{}^{JTS}(r')\}\times\mathcal{Y}_{lSJ}{}^{M}(\mathbf{r})\mathcal{Y}_{l'SJ}{}^{M}(\mathbf{r}')P_T, \tag{3}$$

where μ is the nucleon mass, P_T an isospin projection

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[1] C. Bressel, A. Kerman, and E. Lomon, Bull. Am. Phys. Soc. **10**, 584 (1965).
[2] M. Baranger, *Cargese Lectures in Theoretical Physics* (W. A. Benjamin, Inc., New York, 1963); F. Villars, in *Proceedings of the International School of Physics, "Enrico Fermi," Course 23*, edited by V. F. Weisskopf (Academic Press Inc., New York, 1963).
[3] F. Tabakin, Ann. Phys. (N. Y.) **30**, 51 (1964); Ph.D. thesis, MIT, 1963 (unpublished).
[4] M. K. Pal, A. K. Kerman, and J. P. Svenne, in Proceedings of the International Conference on Nuclear Physics, Gatlinburg, Tennessee, 1966 (to be published).
[5] S. J. Krieger, M. Baranger, and K. T. R. Davies, Nucl. Phys. **84**, 545 (1966).
[6] A. K. Kerman, J. P. Svenne, and F. M. H. Villars, Phys. Rev. **147**, 710 (1966).

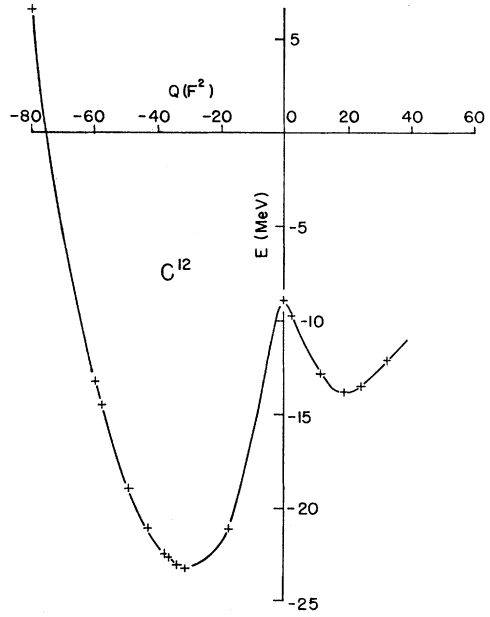

FIG. 1. The Hartree-Fock energy of C^{12} as a function of the deformation. This curve was obtained by adding μQ_{op} to the Hamiltonian and varying μ. A similar behavior appears for all the closed-subshell nuclei.

operator, and l, l' take on the values 0, 1, and 2. The g's and h's have essentially Yukawa shapes, modified by sines and cosines and were adjusted to fit two-body scattering data and

$$\mathcal{Y}_{lsJ}{}^{M}(\mathbf{r})=\sum_{m_l m_S}(lsm_l m_S|JM)Y_l{}^{m_l}(\mathbf{r})\chi_S{}^{m_S}. \quad (4)$$

The Hamiltonian then consisted of the kinetic energy, the Tabakin potential and a center-of-mass correction:

$$H=T+V-P^2/2A\mu. \quad (5)$$

No Coulomb interaction was included so that experimentally observed quantities had to be suitably modified before comparisons were made.

In principle, the Hartree-Fock matrix is infinitely dimensional. Here α and β were taken to be harmonic-oscillator states ($\hbar/\mu\omega=2.6$), and the space consisted of the $1s$, $1p$, $2s$-$1d$, and $2p$-$1f$ shells. The occupied orbitals were also expanded in harmonic oscillators in this space:

$$|\lambda\rangle=\sum|nljm\tau_z\rangle C. \quad (6)$$

The effect of this truncation has been investigated in previous calculations[5,6] for the spherical nuclei. The rapid convergence of the C's is explicitly demonstrated by Krieger *et al.*[5] where, for example, in the lowest state in O^{16} the first two terms account for 99.7% of the solution. This convergence may not be as good for the deformed nuclei, but computer limitations imposed this restriction in all cases.

In order to expand λ in a complete set of states in this truncated space, the summation should include n, l, j, m, and τ_z. In these calculations, m and τ_z were considered fixed so that

$$|\lambda\rangle=\sum_{nlj}|nljm\tau_z\rangle C_{nlj}{}^{m\tau_z}. \quad (7)$$

Previous calculations[7] have shown that the restriction to good m resulted, at most, in a Hartree-Fock energy that was a few MeV above the minimum obtained by varying also m. Since the concern here was mainly the gross properties of nuclei, this extra refinement was sacrificed because of the computational simplification thereby afforded. Preliminary investigations[8] have indicated that for even-even nuclei, there is no advantage to mixing isospin. In fact, it has been shown[9] that the summation on all l, i.e., parity mixing, is not necessary since at the minima the single-particle orbitals do have good parity for the force being used. The calculation is unrestricted in the sense that angular and radial variations are allowed. This is of course a necessity since the deformed even-even nuclei are considered as well as the spherical with A between 4 and 40.

III. HARTREE-FOCK RESULTS

A solution of the Hartree-Fock equations corresponds to a stationary value of the energy. This value may correspond to the absolute minimum, a local minimum, or a maximum. This question can be solved by trying different sets of initial C's or, as was done here, through the use of a Lagrange multiplier. A term μQ was added to the Hamiltonian, where Q is the quadrupole moment operator. Then by letting μ take on a range of values, the energy may be determined as a function of deformation. For example, consider the closed subshell nucleus, C^{12}. If the C's are initially chosen such that the $1s_{1/2}$ and $1p_{3/2}$ orbits are filled (and $\mu=0$) then the re-

TABLE I. The nuclear binding energies as calculated in the Hartree-Fock approximation. E_{HF} represents the Hartree-Fock result, which for a deformed nucleus corresponds to an intrinsic state without good angular momentum. Thus, a moment-of-inertia parameter, $\hbar^2/2I$, taken from experiment, and $\langle J^2\rangle$ are used to obtain the $J=0$ ground state. The Coulomb-corrected observed energies E_{obs} (MeV) and the calculated quadrupole moments Q (barns) are also listed.

Nucleus	E_{HF} (MeV)	$\hbar^2/2I$ (MeV)	$\langle J^2\rangle$	$E^{J=0}$ (MeV)	E_{obs} (MeV)	Q (b)
He^4	−12.78	0	0	−12.78	−28.5	0
Be^8	−12.34	0.52	10.50	−17.57	−59.0	+0.443
C^{12}	−23.17	0.74	8.82	−29.70	−98.6	−0.325
O^{16}	−46.99	0	0	−46.99	−139.5	0
Ne^{20}	−51.78	0.23	18.57	−56.05	−179.2	+0.524
Mg^{24}	−64.72	0.21	17.10	−68.31	−224.7	+0.640
Si^{28}	−86.16	0.25	20.30	−91.23	−272.0	−0.683
S^{32}	−105.38	0.27	14.25	−109.27	−317.3	+0.402
Ar^{36}	−129.82	0.33	6.37	−131.92	−363.4	+0.212
Ca^{40}	−154.73	0	0	−154.70	−410.8	0

[7] J. Bar-Touv and I. Kelson, Phys. Rev. **138**, B1035 (1965).
[8] A. D. MacKellar and W. H. Bassichis (unpublished).
[9] W. H. Bassichis and J. P. Svenne, Phys. Rev. Letters **18**, 80 (1967).

TABLE II. The coefficients of the expansion of the occupied orbitals in the harmonic-oscillator basis. Only the $+m$, $\tau_z=+\frac{1}{2}$ orbitals are listed. The $\tau_z=-\frac{1}{2}$ C's are identical with those listed. The C's for $-m$ can be obtained by using $C_{nlj}{}^{-m\tau_z}=(-1)^{j-m}C_{nlj}{}^{+m\tau_z}$.

Nucleus	(nlj) (in π)	$1s_{1/2}$	$1p_{3/2}$	$1p_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$	$2p_{1/2}$
Be^8	$\frac{1}{2}+$	−0.9633			−0.1987	−0.0177	+0.1795				
	$\frac{1}{2}-$		+0.8463	−0.5046				+0.1315	−0.0055	−0.1050	+0.0272
C^{12}	$\frac{1}{2}+$	+0.9848			−0.1231	+0.0544	+0.1097				
	$\frac{3}{2}-$		+0.9936					−0.0825	+0.0379	+0.0665	
	$\frac{1}{2}-$		−0.7142	−0.6922				+0.0820	−0.0380	+0.0499	−0.0067
O^{16}	$\frac{1}{2}+$	+0.9983				0.0583					
	$\frac{1}{2}-$		−0.9967						−0.0811		
	$\frac{3}{2}-$		+0.9967						+0.0811		
	$\frac{1}{2}-$			−0.9999							−0.0020
Ne^{20}	$\frac{1}{2}+$	−0.9948			−0.0480	−0.0768	+0.0462				
	$\frac{1}{2}-$		+0.9390	−0.3076				+0.1099	+0.0464	−0.0937	+0.0268
	$\frac{3}{2}-$		−0.9916					−0.0318	−0.1227	+0.0260	
	$\frac{1}{2}-$		+0.3155	+0.9436				−0.0262	+0.0526	+0.0705	+0.0399
	$\frac{1}{2}+$	+0.0250			−0.8614	+0.4010	+0.3106				

sult will be spherical with $E=-8.95$ MeV. By varying μ, however, one finds that there exists prolate and oblate solutions with lower energies, −13.80 and −23.17 MeV, respectively; i.e., the spherical solution corresponds to a maximum. Figure 1 shows this behavior of E in deformation space. An identical situation was found in the other closed subshell nuclei in this region, Si^{28} and S^{32}. It is interesting to note that C^{12} has excited 0^+ states at 7.6 and 10.1 MeV, one of which might correspond to the prolate minimum.

If the Hartree-Fock minimal energy is associated with a deformed determinant then direct comparison with experiment is not possible. In such a case, the Hartree-Fock energy corresponds to an intrinsic state which is not an eigenstate of the angular momentum. Projection of eigenstates of J from the intrinsic state can presently be carried out only if A is small[10] so instead a naive rotational correction was made. It was assumed that

$$E_{\mathrm{HF}}=E_{J=0}+(\hbar^2/2I)\langle J^2\rangle \tag{8}$$

so that the experimental binding energies could be obtained if $\hbar^2/2I$, the moment-of-inertia parameter, and the mean value of J^2 were known. The latter quantity is easily calculated from the Hartree-Fock wave function, but although various formulas exist for I, none is considered reliable. Thus, I was taken from the observed spacing in the ground-state rotational band. This is admittedly quite a rough procedure, but the error involved will not appreciably affect the results. Table I contains the Hartree-Fock energies, the mean value of J^2, the approximate value of the moment of inertia parameter, and the resulting calculated binding energies. The experimentally observed binding energies, after subtraction of Coulomb energy,[11] are also listed and, as in Ref. 6, they do not agree with the Hartree-Fock result. It was suggested[6] that the inclusion of second-order effects would offer a solution. That this is, indeed, the situation is shown in the following section. The calculated values of the quadrupole moment,

$$Q_0=(16\pi/5)^{1/2}\langle r^2Y_{20}\rangle, \tag{9}$$

are found in Table I.

Table II contains the expansion coefficients of the occupied orbitals. [See Eq. (7).]

IV. PERTURBATION EXPANSION AND SECOND-ORDER RESULTS

The full Hamiltonian in second quantized notation is

$$H=\sum_{\alpha\beta} t_{\alpha\beta}a_\alpha{}^\dagger a_\beta+\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta}{}^{\gamma\delta}a_\alpha{}^\dagger a_\beta{}^\dagger a_\delta a_\gamma. \tag{10}$$

The Hartree-Fock procedure has supplied a solution to the Schrödinger equation for N particles:

$$H_{\mathrm{HF}}=\sum_{\alpha\beta}(t_{\alpha\beta}+\sum_\lambda V_{\alpha\lambda}{}^{\beta\lambda})a_\alpha{}^\dagger a_\beta. \tag{11}$$

The Hartree-Fock results may therefore be considered the first term in a perturbation expansion where the perturbation is

$$H_1=\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta}{}^{\gamma\delta}a_\alpha{}^\dagger a_\beta{}^\dagger a_\delta a_\gamma-\sum_{\alpha\beta\lambda} V_{\alpha\lambda}{}^{\beta\lambda}a_\alpha{}^\dagger a_\beta. \tag{12}$$

The first-order correction to the Hartree-Fock energy, $\langle H_1\rangle$, vanishes. The second-order contribution to the energy is

$$\Delta E=\sum_i \frac{|\langle i|H_1|\mathrm{HF}\rangle|^2}{E_{\mathrm{HF}}-E_i}, \tag{13}$$

[10] W. H. Bassichis, B. Giraud, and G. Ripka, Phys. Rev. Letters **15**, 980 (1965).

[11] The Coulomb subtraction was accomplished by employing the Coulomb energy expression of D. C. Peaslee [Phys. Rev. **95**, 717 (1954)].

TABLE III. The Hartree-Fock energy with second-order corrections. $E^{J=0}$ is the usual Hartree-Fock result, corrected for rotational energy for the deformed nuclei. E_{total} is the result including second-order contributions. That the second-order contribution is large should not be taken as an indication that the perturbation series does not converge. The second-order contribution is in fact only about 17% of the Hartree-Fock potential energy, indicating convergence.

Nucleus	ΔE_2	$E^{J=0}$	E_{tot}	E_{obs}	E_{tot}/A	E_{obs}/A
He^4	−7.04	−12.78	−19.82	−28.5	−4.96	−7.13
Be^8	−17.57	−17.57	−35.14	−59.0	−4.29	−7.38
C^{12}	−37.57	−29.70	−67.27	−98.6	−5.61	−8.21
O^{16}	−68.46	−46.99	−115.45	−139.5	−7.22	−8.72
Ne^{20}	−94.43	−56.05	−150.48	−179.2	−7.52	−8.96
Mg^{24}	−126.47	−68.31	−694.78	−224.7	−8.12	−9.36
Si^{28}	−159.11	−91.23	−250.34	−272.0	−8.94	−9.71
S^{32}	−197.33	−109.27	−306.60	−317.3	−9.58	−9.92
Ar^{36}	−239.05	−131.92	−370.97	−363.4	−10.35	−10.10
Ca^{40}	−282.99	−154.70	−437.69	−410.8	−10.94	−10.27

where i indicates two-particle two-hole states in the Hartree-Fock basis. An explicit expression for ΔE, using Eq. (12) and the Hartree-Fock wave function, yields

$$\Delta E=\sum_{m<n}\sum_{a,b}\frac{|\langle mn|V|ab\rangle|^2}{\epsilon_m+\epsilon_n-\epsilon_a-\epsilon_b}, \tag{14}$$

where m and n represent occupied states and a and b unoccupied states. Employing various approximations, Pal *et al.*[4] reduced the expression above to a sum of matrix elements, with known coefficients, of the form

$$\langle R_1|V(Q/e)V|R_2\rangle, \tag{15}$$

when R_1 and R_2 are the relative wave functions of two particles, Q is an operator that takes the Pauli principle into account approximately. The propagator e is obtained by assuming plane waves for a and b, with the corresponding energies for ϵ_a and ϵ_b and using a constant that represents an average for the ϵ_m and ϵ_n.

These second-order matrix elements were used to calculate the second-order contribution to the binding energy of all the nuclei considered. Table III contains these results, the sum of the Hartree-Fock energy and the second-order term, this energy with the angular momentum correction, and once again the experimental values. (See also Fig. 2.) In the table the calculated and observed energy per particle is also given. The agreement is now seen to be quite striking. That the perturbation series seems to converge is not obvious when comparing the results in Table III with those in Tables I and II. It is, however, the Hartree-Fock potential energy, not the binding energy, that must be compared with the second-order correction. In O^{16}, for example, the kinetic energy is of the order of 300 MeV, and the Hartree-Fock binding energy is of the order of 50 MeV. Thus, the ratio of the second-order term to the zeroth-order term is about 17%. If this ratio persists in higher order, the agreement would continue to be very satisfactory.

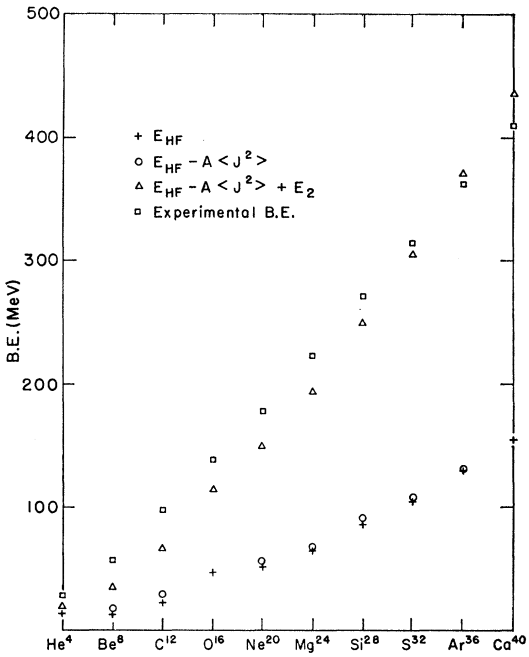

FIG. 2. The Hartree-Fock energy with the angular-momentum correction and the second-order correction compared to the observed binding energies (after Coulomb subtraction). The effect of assuming a constant (independent of A) for Hartree-Fock hole energies [Eq. (14)] could explain the systematic deviation of the corrected results from experiment.

It should be noted that there is a systematic variation of the calculated energies from those observed. This can be directly attributed to the use of a constant-energy denominator in Eq. (15), independent of A. The average value was qualitatively determined from O^{16}, and it is seen to be too large for the lighter nuclei and too small near $A=40$. The results for the single particle energy levels ϵ_a in O^{16} and Ca^{40} (see Ref. 6) show that, in fact, the energy denominator would have the correct dependence if the calculated ϵ's were used instead of an average. Hartree-Fock type calculations can be carried out with effective forces derived from singular potentials.[12] Recent calculations of this type yield results which are also in reasonable agreement with experiment.[13]

V. SINGLE-PARTICLE ENERGIES

Formally, the definition of the single-particle energy levels in a nucleus is unambiguous. For the occupied levels of O^{16}, for example, the energy of the ith level is given by

$$\epsilon_i=E(O^{16})-E^i(O^{15}), \tag{16}$$

where the i indicates a hole in the ith level. The unoccu-

[12] K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. 121, 255 (1961).
[13] C. M. Shakin, M. Tomaselli, T. R. Waghmare, and M. H. Hull (to be published).

TABLE IV. Single-particle energies. ϵ_0 represents the single-particle energy referred to in the text as the Hartree-Fock result: The A-particle Hartree-Fock wave functions are used to calculate the various $A\pm1$ system energies. Δ_P is the change in the ϵ's if the $A\pm1$ energies are calculated self-consistently, allowing them to deform (i.e., be polarized by the additional particle or hole). Δ_2 represents the second-order correction to ϵ_0 for the spherical nuclei and to Δ_P for the deformed nuclei. $\hat{\epsilon}_2$ is just $\epsilon_0+\Delta_P+\Delta_2$. The single-particle states are labeled by their only quantum numbers, m and π. The quantum numbers of the "parent level," i.e., the dominant term in the expansion of λ, are also given for the spherical nuclei. In principle, the energies of the $A\pm1$ nuclei in the spherical cases and of all the nuclei in the deformed cases should be the results of projecting, not the intrinsic energy as shown. This introduces an error into all the single-particle results, which is probably small but could not be accurately estimated. Since the deformation is some measure of the size of the correction, those systems with large deformation are starred.

	(nlj)	$(m\pi)$	ϵ_0	Δ_P	Δ_2	$\hat{\epsilon}_2$	ϵ_{obs}
				He^4			
occupied	$1s_{1/2}$	$\frac{1}{2}+$	−14.73	+1.17	−3.46	−17.02	−20
unoccupied	$1p_{3/2}$	$\frac{1}{2}-$	+8.98	−0.46	−1.66	+6.96*	+1
	$1d_{5/2}$	$\frac{1}{2}+$	+15.96	−0.01	−1.71	+14.24*	+20
	$1f_{7/2}$	$\frac{5}{2}-$	+28.22	−0.17	−1.03	+26.16*	
				O^{16}			
occupied	$1s_{1/2}$	$\frac{1}{2}+$	−45.42	+3.73	−10.31	−52.00	−44
	$1p_{3/2}$	$\frac{3}{2}-$	−19.73	+0.90	−7.76	−26.59*	−22
	$1p_{1/2}$	$\frac{1}{2}-$	−9.74	+0.23	−8.39	−17.90	−15.7
unoccupied	$1d_{5/2}$	$\frac{1}{2}+$	+2.93	−0.09	−5.18	−2.34	−4.15
	$2p_{3/2}$	$\frac{1}{2}-$	+18.33	−0.09	−5.31	+12.93	
	$1f_{7/2}$	$\frac{7}{2}-$	+18.25	−0.13	−3.74	+14.38*	
				Ca^{40}			
occupied	$1p_{3/2}$	$\frac{3}{2}-$	−48.13	+0.04	−15.01	−62.74*	−45?
	$1p_{1/2}$	$\frac{1}{2}-$	−34.92	+0.14	−16.10	−50.88	−33?
	$1d_{5/2}$	$\frac{5}{2}+$	−23.76	+0.11	−11.50	−35.15*	−22.8
	$1d_{3/2}$	$\frac{3}{2}+$	−6.41	+0.09	−13.60	−19.92*	−15.8
unoccupied	$1f_{7/2}$	$\frac{1}{2}-$	−1.81	−0.02	−9.10	−10.93*	−8.37
				Be^8			
occupied		$\frac{1}{2}+$	−21.60	+4.46	−9.24	−26.38	
		$\frac{1}{2}-$	−9.87	+0.63	−4.69	−13.93	−18.5
unoccupied		$\frac{3}{2}-$	+3.95	−0.17	−2.31	+1.42	−1.7
		$\frac{1}{2}-$	+7.07	−0.29	−2.18	+4.60	+6.2?
		$\frac{1}{2}+$	+10.68	−0.44	−3.43	+6.81	0
		$\frac{3}{2}+$	+13.77	−0.24	−2.49	+11.04	
		$\frac{5}{2}+$	+18.09	−0.11	−1.83	+16.15	
		$\frac{5}{2}-$	+25.49	−0.30	−1.02	+24.17	
		$\frac{7}{2}-$	+28.48	−0.07	−1.06	+27.35	
				C^{12}			
occupied		$\frac{1}{2}+$	−34.05	+4.25	−11.62	−41.42	−34
		$\frac{3}{2}-$	−13.74	+0.58	−6.21	−19.37	−18.7
		$\frac{1}{2}-$	−11.28	+0.35	−6.24	−17.17	−14
unoccupied		$\frac{1}{2}-$	+1.38	−0.75	−3.68	−3.05	−4.9
		$\frac{5}{2}+$	+6.10	−0.19	−4.05	+1.86	−1.1
		$\frac{3}{2}+$	+9.58	−0.45	−4.06	+5.07	
		$\frac{1}{2}+$	+9.62	−0.57	−5.18	+3.87	
		$\frac{7}{2}-$	+19.67	−0.16	−3.11	+16.40	
		$\frac{3}{2}-$	+19.91	−0.16	−4.25	+15.50	
		$\frac{5}{2}-$	+12.88	−0.06	−2.91	+18.91	
				Ne^{20}			
occupied		$\frac{3}{2}-$	−22.68	+0.94	−10.19	−31.81	
		$\frac{1}{2}-$	−14.91	+0.92	−10.80	−24.74	
		$\frac{1}{2}+$	−6.69	+0.35	−7.82	−14.16	−16.9
unoccupied		$\frac{3}{2}+$	−0.73	−0.26	−6.09	−7.08	−6.8
		$\frac{5}{2}+$	+1.55	−0.15	−5.50	−4.10	−6.5
		$\frac{1}{2}+$	+4.81	−0.27	−7.36	−2.82	−4.0
		$\frac{1}{2}-$	+12.47	−0.36	−6.16	+5.95	
		$\frac{3}{2}-$	+13.89	−0.28	−4.85	+8.76	
		$\frac{5}{2}-$	+16.59	−0.12	−4.31	+12.16	
		$\frac{7}{2}-$	+17.83	−0.10	−3.87	+13.86	

pied levels are similarly given by

$$\epsilon_i = E^i(O^{17}) - E(O^{16}). \quad (17)$$

There are, however, two ways of calculating ϵ_i in the Hartree-Fock framework. These two methods yield different results and have different interpretations.

The first method will be called the Hartree-Fock method. Here the single-particle wave functions resulting from the Hartree-Fock calculation for the A system (O^{16}, for example) are used to calculate the energy of the $A-1$ and $A+1$ system (i.e., O^{15}, O^{17}) as follows:

$$E^i(A\pm1) = \sum_\lambda \langle\lambda|\, t_\lambda a_\lambda^\dagger a_\lambda\,|\lambda\rangle + \tfrac{1}{2}\sum_{\lambda\mu}\langle\lambda\mu|\, V_{\lambda\mu}{}^{\lambda\mu}\,|\lambda\mu\rangle, \quad (18)$$

where μ and λ represent the single-particle wave functions of the A system, and the summations exclude the ith state if it were originally occupied and include it if it were initially unoccupied. The potential can be either just the Tabakin potential or it may include the second-order matrix elements. The two single-particle energies obtained using Eqs. (16), (17), and (18) will be referred to as $\epsilon_0{}^i$ and $\epsilon_2{}^i$ for straight Hartree-Fock or second order. If the Hamiltonian being considered were $H=T+V$ without the center-of-mass correction, the ϵ_0's would correspond to those in Eq. (2).

An alternative approach is to calculate the HF energy of the $A\pm1$ systems self-consistently and then to add a second-order contribution. This contribution is obtained as the difference of $\epsilon_2{}^i$ and $\epsilon_0{}^i$ above and is called $\Delta_2{}^i$. The single-particle energies calculated in this way will be called the polarization results, $\hat{\epsilon}_0{}^i$ and $\hat{\epsilon}_2{}^i$.

The ϵ's calculated by the first approach are actually the Hartree-Fock single-particle energies which enter into certain procedures, such as the random-phase approximation (RPA) or the BCS approximation. On the other hand, the $\hat{\epsilon}$'s have a more physical interpretation. They include the effect on the single-particle state of the polarization of the core. Since our Hartree-Fock procedure allows any even-parity deformation, this includes the effects of virtual emission and reabsorption of any even-parity multipoles. Since the Hartree-Fock solution for the O^{17} system is deformed, the intrinsic state given by Hartree-Fock should be operated on by projection operators to produce states with sharp angular momentum. The difference between the energies of these projected states and $E(O^{16})$ would then be compared with experiment. In the absence of a practical method of projection for a number of particles as large as 17, the polarization results derived from the intrinsic states of O^{17} serve as an approximation to the projected results. In a sense, the Hartree-Fock ϵ's taken from O^{16} can be considered a further approximation where the polarization of the original particles due to the presence of a particle or hole is neglected.

The results of the two methods are tabulated in Table IV. The differences between the ϵ's and $\hat{\epsilon}$'s are, in most cases, small. For comparison, some experimental values are also listed. Certain, perhaps interesting, single-particle energies do not appear because technical details of the computer programs made it impossible to calculate them.

TABLE V. The symmetry energy as calculated in Hartree-Fock and by the empirical formula. E_{HF} represents the Hartree-Fock result for the binding energy and Δ_{HF} the symmetry energy obtained from these results. E_1 is calculated, using in all cases the Ca^{48} wave functions to calculate the energy of the other $A=48$ systems, and Δ_1 represents the symmetry energy thus obtained. E_{1+2} is calculated in the same way, but the second order contribution is added to the Hamiltonian of the $A=48$ system. E_{HF+2} represents the Hartree-Fock results with the second-order perturbation correction added. The empirical values were obtained from formula (19).

	Binding energies (MeV)			
	E_{HF}	E_1	E_{1+2}	E_{HF+2}
Cr^{48}	−188.66	−185.41	−549.35	−554.74
Ti^{48}	−183.79	−182.30	−544.62	−547.03
Ca^{48}	−175.45	−175.45	−534.62	−534.46

	Symmetry energies (MeV)				
	Δ_{HF}	Δ_1	Δ_{1+2}	Δ_{HF+2}	$\Delta_{empirical}$
Cr^{48}	0	0	0	0	0
Ti^{48}	+4.87	+3.11	+4.73	+7.71	+6.03
Ca^{48}	+13.21	+9.96	+14.89	+20.28	+24.12

VI. SYMMETRY ENERGY

According to the semiempirical mass formula,[14] there should be a variation in the binding energy of isobars independent of Coulomb effects. This variation is called the symmetry energy and is given by[15]

$$E_{sym} = (C/A)(N-Z)^2. \quad (19)$$

The empirical value of C is 18.1 MeV. There is another factor entering into the energy difference between isobars if odd-odd configurations are considered as well as even-even. Therefore, to isolate the symmetry effect, only even-even nuclei are considered.

The $A=48$ system was studied, and the Hartree-Fock energy was calculated for Ca^{48}, Ti^{48}, and Cr^{48}. The results are shown in Table V along with the values computed from the above formula. The agreement is very satisfying in view of the fact that for Ca^{48} the even-parity levels in the space are completely filled so that only twelve of the twenty-eight orbitals can be varied.

VII. CONCLUSIONS

The calculations reported here are preliminary. The object was to test the validity of the Hartree-Fock theory when applied to finite nuclei, starting from a force obtained from two-body scattering data and doing as completely as possible a self-consistent calculation.

[14] C. F. von Weizsäcker, Z. Physik **96**, 431 (1935).

[15] See, for example, J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952), p. 226.

The conclusions are rather apparent. Though some calculated quantities are not consistent with experiment, the over-all agreement is quite reasonable when second-order corrections are taken into account. Since the onset of these calculations, there has been considerable improvement in the smooth, two-body potentials available. It is hoped that these improved potentials will lead to more accurate Hartree-Fock results, and calculations with the newer potentials are beginning. The results reported here are themselves considered sufficiently enlightening so that the Tabakin force is being utilized in calculations in a greatly enlarged space—from the $1s_{1/2}$ to the $1i_{13/2}$. This will permit investigation of heavier nuclei, in fact, up to Pb^{208} and will test the crucial dependence of the present results on the space truncation for deformed nuclei. A method for extracting more accurate information from the intrinsic state of a deformed nucleus, when the number of particles involved renders present projection techniques inapplicable, is being sought.

Work is also in progress to extract from the Hartree-Fock results reported information about the effective nuclear force and other nuclear properties, such as compressibility.

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Radiative Capture of ^{3}He by ^{3}He†

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The reaction $^3He+^3He \rightarrow {}^6Be^*+\gamma$ was observed at 90° for bombarding energies between 0.86 and 11.8 MeV. The total cross section for transitions to the first excited state of ^{6}Be varies smoothly from 0.4 to 9.3 μb (assuming isotropy). No γ-ray transitions to the ground state of ^{6}Be were observed with an upper limit of approximately 10^{-2} μb at 1.4 MeV. Because of these low cross sections, this reaction is of negligible astrophysical importance compared to the $^3He(^3He,2p)^4He$ reaction.

INTRODUCTION

HELIUM-3 capture γ-ray reactions have been observed in several nuclei.[1,2] The capture reaction $^3He+^3He \rightarrow {}^6Be+\gamma$ is a possible way of closing the proton chain of stellar energy production since ^{6}Be breaks up into two protons and an α particle.[3] We have observed this reaction and report here measurements of its yield.

LOW-ENERGY MEASUREMENTS

For the measurements from 1.0- to 1.8-MeV incident energy, a $^3He^+$ beam from the 3-MV Kellogg Radiation Laboratory electrostatic generator was used. The beam entered the 25-cm gas scattering chamber (see Fig. 1) through a differentially pumped canal in which the ^{3}He gas pressure in the chamber could be dropped by more than a factor of 100. The ^{3}He gas in the system was recirculated and passed through a liquid-nitrogen-cooled molecular sieve trap for purification before again entering the target chamber.[4] Stable gas pressures from 13 to 16 Torr were used in the chamber. The beam current, typically 1 to 2 μA, was collected in a thermally insulated low-mass metal cup. Beam power was measured by balancing the collector-cup temperature with a nearby dummy cup of the same geometry but heated electrically. The beam particle flux was then obtained from the integrated electric power dissipated in the dummy cup, after correcting the beam energy for energy loss in the target gas.[4]

A 10-cm-diam by 10-cm-thick NaI(Tl) crystal was introduced into a well in the gas chamber so that its front face was 4.1 cm from the beam line. The beam was completely surrounded by a tantalum shield in order to reduce the background of secondary neutrons produced by the high-energy protons from the $^3He(^3He,2p)^4He$ reaction. The crystal was shielded with lead from both the tantalum entrance canal and the collecting cup. Additional shielding was used to reduce the neutron

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[1] P. D. Parker and R. W. Kavanagh, Phys. Rev. **131**, 2578 (1963); D. Kohler and S. M. Austin, Bull. Am. Phys. Soc. **8**, 290 (1963); P. Paul, S. L. Blatt, and D. Kohler, Phys. Rev. **137**, B493 (1965); F. Nüsslin, H. Werner, and J. Zimmerer, Z. Naturforsch. **21**, 1195 (1966).
[2] J. M. Blair, N. M. Hintz, and D. M. Van Patter, Phys. Rev. **96**, 1023 (1954).
[3] P. D. Parker, J. N. Bahcall, and W. A. Fowler, Astrophys. J. **139**, 602 (1964).
[4] H. Winkler (to be published).