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HARTREE-FOCK CALCULATIONS WITH WOOD-SAXON BASIS FUNCTIONS

by William F. Ford and Richard C. Braley

Lewis Research Center
Cleveland, Ohio

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ABSTRACT

The Hartree-Fock method is used to study the even-even N Z nuclei in the 2s-1d shell. Basis functions with correct asymptotic behavior are generated by use of a Wood-Saxon well. The results are compared with calculations using the conventional harmonic oscillator basis. It is found that most of the Wood-Saxon results may be obtained with a harmonic oscillator basis if the oscillator parameter is carefully chosen.

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SUMMARY

In order to determine the sensitivity of various nuclear properties to the asymptotic part of the nuclear wave function, calculations have been made using both the conventional harmonic oscillator single-particle functions and the more realistic Wood-Saxon functions. Hartree-Fock theory was used to obtain nuclear wave functions for the five even-even $N = Z$ nuclei in the 2s-1d shell. Intrinsic nuclear energies, radii, and quadrupole moments were calculated, as well as energy gaps and single-particle densities. Considerable differences between harmonic oscillator and Wood-Saxon results were found when the usual value ($\nu = 0.35\ \mathrm{fm}^{-2}$) for the oscillator parameter was used; however, close agreement could be obtained in most of the properties studied by using a different value ($\nu = 0.27\ \mathrm{fm}^{-2}$).

INTRODUCTION

In recent years the Hartree-Fock (HF) method has received considerable attention in studies of the energy levels of deformed nuclei (ref. 1). This method is essentially a variational procedure, based on minimization of the energy of a many-particle system. While such a procedure may provide a sensitive test of the wave function in the nuclear interior, it is expected that the shape of the wave function beyond the nuclear surface will not affect nuclear energies significantly. For this reason, HF calculations up until now have made use of single-particle harmonic oscillator basis functions, in spite of their obviously incorrect asymptotic behavior.

There are, however, many quantities of interest which are expected to be much more sensitive than the total energy to the asymptotic part of the wave function. Electromagnetic transition rates, multipole moments, and form factors for elastic and inelastic scattering are examples which come readily to mind. It does not seem likely that very accurate calculations of such quantities can be performed using HF wave functions with a harmonic oscillator basis. Thus, a HF calculation using the basis functions of the more

realistic Wood-Saxon potential is of interest both for the energy spectrum it yields and for the effect it shows of the long-range part of the wave function on other nuclear properties.

In this report are presented the results of a considerably restricted version of such a program. The HF variational calculation is carried out for five nuclei in the 2s-1d shell by using both Wood-Saxon (WS) and harmonic oscillator (HO) basis functions. A comparison is made of such properties as orbital energies, energy gap, and total (HF) energy. In addition, nuclear densities, radii, and intrinsic quadrupole moments are calculated and compared.

SYMBOLS

a	diffuseness of Wood-Saxon well
C_a^λ	expansion coefficients for the Hartree-Fock orbits
E_{HF}	Hartree-Fock energy
e_λ	Hartree-Fock single-particle energy
h	Hartree-Fock Hamiltonian
h_o	independent-particle Hamiltonian
$\hat{J}$	$\sqrt{2J + 1}$
(jm)	single-particle total angular momentum and its projection onto z-axis
$\langle j_1 m_1, j_2 m_2 \vert JM\rangle$	Clebsch-Gordan coefficient
$\langle j' \vert\vert T_J \vert\vert j\rangle$	reduced matrix element
l_a	single-particle orbital angular momentum
$\begin{Bmatrix} l_a & s_a & j_a \\ l_b & s_b & j_b \\ L & S & J \end{Bmatrix}$	symmetric 9-j coefficient
$\binom{n}{m}$	$\dfrac{n!}{m!(n - m)!}$
P_{ij}	two-particle exchange operator
r_{ij}	$\lvert \vec{r}_i - \vec{r}_j \rvert$

(SM_S)	total spin angular momentum and projection onto z-axis
$U(j_1j_2j_4j_3;J_{12}J)$	U-coefficient of Jahn (see ref. 9); defined in terms of Racah coefficient as $[(2J_{12}+1)(2J+1)]^{1/2}W(j_1j_2j_4j_3;J_{12}J)$
$u_a(i)$	$u_a(r_i)Y_{l_a 1/2 j_a}^{m_a}(i)X_{1/2}^{\tau}(i)$
$u_a(r_i)$	radial part of basis function
$V(ij)$	residual two-body force
V_o	strength of residual two-body force and/or Wood-Saxon well
$v(i)$	nonlocal part of the Hartree-Fock Hamiltonian
$W(j_1j_2j_4j_3J_{12}J)$	Racah coefficient
$Y_L^m(i)$	spherical harmonic
$Y_{l\,sj}^m(i)$	$\sum_{m_1m_2} \langle l\,m_1, sm_2 \vert jm\rangle\ Y_l^{m_1}(i)X_s^{m_2}(i)$
Δ	energy gap between occupied and unoccupied orbits
μ	nucleon-nucleon force range
ν	Harmonic oscillator parameter
$\rho(r)$	single-particle density function which includes core effects
$\rho_v(r)$	single-particle density function for valence particles only
$\vec{\sigma}(i)$	Pauli spin operator for particle i
τ_a	z-projection of single-particle isotopic spin
$\int d\tau_j$	integral over all coordinates of jth particle
Φ	determinantal wave function for A-particle system
$\varphi_\lambda(i)$	Hartree-Fock orbital function of ith particle
χ_{SM_S}	total spin wave function for two-particle system
$\chi_S^m(i)$	spin wave function for i^{th} particle
$\chi_{1/2}^{\tau}(i)$	isospin function for i^{th} particle

THEORY

In the HF method, the nuclear wave function is approximated by the Slater determinant

$$\Phi = (A!)^{-1/2} \det \{\varphi_\lambda(i)\} \tag{1}$$

whose orbital functions $\varphi_\lambda(i)$ are determined by minimizing the expectation value of the nuclear Hamiltonian. This variational problem leads to the eigenvalue equation

$$h\varphi_\lambda = (h_o + v)\varphi_\lambda = \epsilon_\lambda \varphi_\lambda \tag{2}$$

where

$$v(i) = \frac{1}{2} \sum_\mu \int d\tau_j \varphi^*_\mu(j) V(ij)(1 - P_{ij})\varphi_\mu(j) \tag{3}$$

The operator h_o is usually taken to be the Hamiltonian for a single nucleon moving in the average nuclear field, and V represents the residual two-body force. The presence of the exchange operator P_{ij} is a natural consequence of the antisymmetry of the determinant. The summation in equation (3) is taken over all the orbits which are to be varied.

Since equations (2) and (3) are too difficult for a direct solution, approximation methods are required. Usually one begins by selecting a suitable set of basis functions and then making the expansion

$$\varphi_\lambda(i) = \sum_a C^\lambda_a u_a(i) \tag{4}$$

The problem then reduces to diagonalizing h in the space spanned by the basis functions u_a. In practice, this is accomplished in an approximate way by first truncating the space, then guessing at an initial set C^λ_a, and finally iterating until two successive diagonalizations yield the same set C^λ_a. (Often "a" will be written for the set $j_a m_a$, the set j_a, or even the set $n_a l_a j_a$ when no confusion will result.)

In order to carry out this procedure, one needs matrix elements of h. It is generally assumed that h_o is diagonal with eigenvalues deduced from experimental spectra. The matrix elements of v may be expressed (ref. 1) in terms of the coupled two-body

matrix elements of V:

$$\langle a|v|c\rangle = \frac{1}{2} \sum_{\mu} \sum_{bd} \left(C_b^{\mu *} C_d^{\mu}\right) \sum_{JT} \langle j_a m_a, j_b m_b | JM\rangle \langle j_c m_c, j_d m_d | JM\rangle$$

$$\times \left\langle \frac{1}{2} \tau_a, \frac{1}{2} \tau_b | TM_T \right\rangle \left\langle \frac{1}{2} \tau_c, \frac{1}{2} \tau_d | TM_T \right\rangle \langle ab | V | \widetilde{cd}\rangle_{J_T} \tag{5}$$

(The tilde indicates that the product function $u_c(i)u_d(j)$ has been antisymmetrized.) The two-body matrix elements $\langle ab|V|\widetilde{cd}\rangle_{JT}$ are of course independent of the orbital functions, and they are therefore ideally suited for use as input in a general program designed to solve equation (2).

Calculation of the two-body matrix elements presents some problems which stem from the fact that V(ij) is a function of the separation between nucleons i and j. If HO functions are used, one can overcome the difficulty by transforming to center-of-mass and relative coordinates, and the resulting integrals can be expressed in terms of Moshinsky brackets (ref. 2). In the general case, however, such a transformation is not possible, and the most promising approach seems to be an expansion of V(ij).

For the moment the isotopic spin dependence is ignored. The coupled matrix element may then be written

$$\langle ab | V | \widetilde{cd}\rangle_J = \left\langle \varphi_{JM}^{ab}(12) \left| V(12) \right| \varphi_{JM}^{cd}(12) - \varphi_{JM}^{cd}(21) \right\rangle \tag{6}$$

where

$$\varphi_{JM}^{ab}(12) = \sum_{m_a m_b} \langle j_a m_a, j_b m_b | JM\rangle u_a(1) u_b(2) = (-1)^{j_a + j_b - J} \varphi_{JM}^{ba}(21) \tag{7}$$

After switching from j - j to L - S coupling (ref. 3) by means of

$$\varphi_{JM}^{ab} = \sum_{M_L M_S} \langle LM_L, SM_S | JM\rangle \varphi_{LM_L}^{ab} \chi_{SM_S}$$

we obtain

$$\left\langle \varphi^{ab}_{JM}(12) \,|\, V(12) \,|\, \varphi^{cd}_{JM}(ij) \right\rangle = \sum_{LS} Q^{ab}_{LSJ} Q^{cd}_{LSJ}$$

$$\times \left\langle \varphi^{ab}_{LM_L}(12)\chi_{SM_S}(12) \,|\, V(12) \,|\, \varphi^{cd}_{LM_L}(ij)\chi_{SM_S}(ij) \right\rangle \tag{8}$$

where $M_L + M_S = M$ and

$$Q^{ab}_{LSJ} \equiv \hat{L}\hat{S}\hat{j}_a\hat{j}_b \begin{Bmatrix} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ L & S & J \end{Bmatrix} \tag{9}$$

In this derivation V is assumed invariant under space and spin rotations separately. Usually a spin dependence of the form

$$V(12) = \sum_{S'=0}^{1} V_{S'}(12)\vec{\sigma}_{S'}(1) \cdot \vec{\sigma}_{S'}(2) \tag{10}$$

is also assumed where $\vec{\sigma}_0$ is the unit operator in spin space and $\vec{\sigma}_1$ is the ordinary Pauli spin operator. Then, since $\chi_S(12) = (-1)^{1+S}\chi_S(21)$,

$$\langle ab|V|\widetilde{cd}\rangle_J = \sum_{LS} Q^{ab}_{LSJ} Q^{cd}_{LSJ} \sum_{S'} A_{SS'}$$

$$\times \left\langle \varphi^{ab}_{LM}(12) \,|\, V_{S'}(12) \,|\, \varphi^{cd}_{LM}(12) + (-1)^S \varphi^{cd}_{LM}(21) \right\rangle \tag{11}$$

where

$$A_{SS'} \equiv \langle S|\,|\vec{\sigma}_{S'}(1) \cdot \vec{\sigma}_{S'}(2)|\,|S\rangle$$

$$= 2(2S' + 1)(-1)^{S-1} W\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\middle|S'S\right) = 1 - 4\delta_{S0}\delta_{S'1} \tag{12}$$

Next the spherical harmonics in φ^{ab}_{LM} and φ^{cd}_{LM} are decoupled and then recoupled according to

$$Y^*_{l_a m_a}(1) Y_{l_c m_c}(1) = \sum_{L'M'} \langle l_a || Y_{L'} || l_c \rangle \langle l_c m_c, L'M' | l_a m_a \rangle Y^*_{L'M'}(1) \tag{13a}$$

$$Y^*_{l_b m_b}(2) Y_{l_d m_d}(2) = \sum_{L''M''} \langle l_d || Y_{L''} || l_b \rangle \langle l_b m_b, L''M'' | l_d m_d \rangle Y_{L''M''}(2) \tag{13b}$$

Now, after a little more Racah algebra, the coupled matrix element may be written

$$\langle ab | V | \tilde{cd} \rangle_J = \sum_{LS} Q^{ab}_{LSJ} Q^{cd}_{LSJ} \sum_{L'S'} A_{SS'} \Big[B^{ac,db}_{LL'} F^{ac,db}_{L'S'} + (-1)^{L+S+l_c+l_d} B^{ad,cb}_{LL'} F^{ad,cb}_{L'S'} \Big] \tag{14}$$

where

$$B^{ac,db}_{LL'} \equiv \langle l_a || Y_{L'} || l_c \rangle \langle l_b || Y_{L'} || l_b \rangle U(l_c L' L l_b | l_a l_d) \tag{15}$$

$$F^{ac,db}_{LS} = \left\langle \varphi^{ac}_{LM}(1) | V_s(12) | \varphi^{db}_{LM}(2) \right\rangle \tag{16}$$

and

$$\varphi^{ac}_{LM}(1) \equiv u_a(r_1) u^*_c(r_1) Y_{LM}(\hat{r}_1) \tag{17}$$

In the derivation of equation (14) V_S is assumed central so that the sums over L'' and M'' reduce to a single term.

The final step is the inclusion of isotopic spin dependence. It is assumed that

$$V_{S'}(12) = \sum_{T'=0}^{1} V_{S'T'}(12) \vec{\tau}_{T'}(1) \cdot \vec{\tau}_{T'}(2) \tag{18}$$

where $\vec{\tau}_0$ and $\vec{\tau}_1$ are defined like $\vec{\sigma}_0$ and $\vec{\sigma}_1$ but in isotopic spin space. The treatment is evidently exactly like that given for the spin dependence. With the customary assumption that

$$V_{S'T'}(12) = \beta_{S'T'} V(|\vec{r}_1 - \vec{r}_2|) \tag{19}$$

where $\beta_{S'T'}$ measures the relative strengths of $V_{S'T'}$, the final result is obtained:

$$\langle ab|V|\tilde{cd}\rangle_{JT'} = \sum_{LS} Q^{ab}_{LSJ} Q^{cd}_{LSJ} \sum_{L'S'T'} A_{SS'} A_{TT'} \beta_{S'T'} \left[B^{ac,\,db}_{LL'} F^{ac,\,db}_{L'} - (-1)^{L+S+T+l_c+l_d} B^{ad,\,cb}_{LL'} F^{ad,\,cb}_{L'} \right] \tag{20}$$

where

$$F^{ac,\,db}_{L} = \left\langle \varphi^{ac}_{LM}(1) \,|\, V \,|\, \varphi^{db}_{LM}(2) \right\rangle \tag{21}$$

The method used to evaluate integral (21) is based on a technique due to Sawaguri and Tobocman (ref. 4), who developed a general formalism for evaluation of six-dimensional integrals. A simplified version adequate for the work herein is obtained as follows. Let

$$f_{l\,mn}(\vec{r}) \equiv \mathcal{F}^{l}_{n}(r) Y_{l\,m}(\hat{r}) \tag{22}$$

be a complete set of functions in terms of which the expansion

$$V(|\vec{r} - \vec{r}_2|) = \sum_{\substack{l\,m \\ n_1 n_2}} V_{n_1 n_2 l} f_{l\,mn_1}(\vec{r}_1) f^{*}_{l\,mn_2}(\vec{r}_2) \tag{23}$$

is made. The desired integral (21) may then be written

$$F^{ac,\,db}_{L} = \sum_{n_1 n_2}^{\infty} V_{n_1 n_2 L} F^{ac}_{n_1 L} \left(F^{db}_{n_2 L} \right)^{*} \tag{24}$$

where

$$F_{nL}^{ac} = \int_0^\infty u_a^*(r)\mathscr{F}_n^L(r)u_c(r)r^2\,dr \tag{25}$$

The usefulness of the method depends on whether the series in equation (24) is rapidly convergent and whether values of $V_{n_1n_2l}$ are easy to obtain. Sawaguri and Tobocman showed that for the choice

$$\mathscr{F}_n^l(r) = \mathscr{F}_n^l(\alpha,\beta r) \equiv \frac{1}{n!}\,(\beta r)^l\,e^{-\alpha^2\beta^2r^2/2}\,{}_1F_1(-n;l + 3/2;\beta^2r^2) \tag{26}$$

one gets

$$V_{n_1n_2l} = \sum_{m_1=0}^{n_1}\sum_{m_2=0}^{n_2} G_{m_1n_1}^l G_{m_2n_2}^l V_{m_1+m_2+l} \tag{27}$$

where

$$V_m = \pi\left(\frac{2\beta}{\sqrt{2-\alpha}}\right)^3 \frac{\Gamma\left(m+\frac{3}{2}\right)}{(-\alpha)^m}\int_0^\infty V(r)\mathscr{F}_m^0\left(2,\ \frac{\sqrt{2-\alpha}}{2}\beta r\right)r^2\,dr \tag{28}$$

and

$$G_{mn}^l = \left(\frac{-\alpha}{2-\alpha}\right)^{n+l/2}\binom{n}{m}\frac{\Gamma\left(n+l+\frac{3}{2}\right)}{\Gamma\left(l+\frac{3}{2}\right)\Gamma\left(m+l+\frac{3}{2}\right)} \tag{29}$$

In practice, for appropriate choices of α and β, the series in equation (24) can be made to converge sufficiently fast to make the entire scheme an excellent computational device.

RESULTS

The theory just described has been applied to the five s-d shell nuclei neon 20, magnesium 24, silicon 28, sulfur 32, and argon 36 (Ne^{20}, Mg^{24}, Si^{28}, S^{32}, and A^{36}). The HF wave functions are assumed to have axial symmetry (ref. 5), and they are formed by

putting particles into deformed orbits about a spherical, closed-shell, inert oxygen 16 (O^{16}) core. Each deformed orbit is described as a mixture of $1d_{5/2}$, $2s_{1/2}$, and $1d_{3/2}$ basis vectors, each with the appropriate spin projection m_λ. The coefficients for the negative m_λ orbits are related to those for the positive m_λ orbits by time reversal symmetry:

$$C_j^\lambda(-m_\lambda) = C_j^\lambda(m_\lambda)(-1)^{j-m_\lambda} \tag{30}$$

The eigenvalues of h_o used in the calculation are taken from the experimental spectrum of oxygen 17 (O^{17}), and they are listed in the fourth column of table I. The residual two-body force $V(ij)$ is a Rosenfeld mixture with Gaussian shape, much like that used by Ripka (ref. 1):

$$V(ij) = V_o \frac{\vec{\tau}_i \cdot \vec{\tau}_j}{3} \left[0.3 + 0.7\, \vec{\sigma}_1(i) \cdot \vec{\sigma}_1(j)\right] e^{-\mu r_{ij}^2} \tag{31}$$

with $V_o = -50$ MeV (instead of Ripka's $V_o = -55$ MeV) and $\mu = 0.29$ per square femtometer (fm^{-2}).

For a discussion of the basis vectors themselves, two sets of harmonic oscillator basis functions were used and one set of Wood-Saxon basis functions (ref. 6). The latter were chosen by varying the parameters V_o and α in the Wood-Saxon potential

$$V = \rho(r) - \alpha\left(\frac{\hbar}{2mc}\right)^2 \vec{\sigma} \cdot \vec{l}\, \frac{1}{r} \frac{d\rho}{dr} \tag{32}$$

$$\rho(r) = \frac{V_o}{\left[1 + \exp\left(\frac{r - R}{a}\right)\right]} \tag{33}$$

so as to reproduce as closely as possible the experimental eigenvalues of h_o as given in table I. The eigenvalues thus obtained are given in the third column of table I.

Choosing the harmonic oscillator basis functions poses something of a problem - namely, what criteria to use. At length it was decided that one set of functions (HO - 1) should be chosen on the basis of similarity to the Wood-Saxon basis functions within the nuclear interior, as measured by comparison of eigenvalues and location of peaks and nodes in the functions. For this set an optimum choice was $\nu = 0.35\ fm^{-2}$. This choice ν is based on an approximate method for calculating the "correct" nuclear radius (ref. 7).

TABLE I. - OXYGEN 17 SINGLE-PARTICLE ENERGIES

Orbit	Energy, MeV			
	Harmonic oscillator parameter, ν, fm^{-2}		Wood-Saxon	Experiment
	$\nu = 0.27\ fm^{-2}$	$\nu = 0.35\ fm^{-2}$		
$1s_{1/2}$	-26.2	-32.6	-34.68	~-35
$1p_{3/2}$	-15.0	-18.2	-20.21	-21.83
$1p_{1/2}$	-15.0	-18.2	-16.53	-15.67
$1d_{5/2}$	-3.7	-3.7	-6.02	-4.14
$2s_{1/2}$	-3.7	-3.7	-4.54	-3.27
$1d_{3/2}$	-3.7	-3.7	-0.53	0.94

A second set (HO - 2) was chosen eventually on the basis of similarity to the Wood-Saxon basis functions as measured by comparison of the resulting nuclear binding energies, orbital energies, energy gaps, and intrinsic quadrupole moments. For this set, $\nu = 0.27\ fm^{-2}$.

In table I the energy eigenvalues of the various basis functions are compared, while in figures 1 to 5 their shapes are compared. Little can be determined from the energy eigenvalues, but figures 1 to 5 reveal clearly for the 1s-ip shell functions that HO-1 is closer to WS than HO-2 is. In the 2s-1d shell the situation is somewhat ambiguous: HO - 1 has the same peaks and nodes as WS, as before, whereas HO-2 has different peaks and nodes but has perhaps an overall better match in magnitude.

The results of HF calculations using the three sets of basis functions just described are compared in tables II(a) and (b). On the basis of the binding energies and the gaps, it is evident that HO-2 gives a better match to the WS results than HO-1.

Root-Mean-Square Radii

The rms radii are obtained from evaluation of the expectation value of the operator

$$\vec{R}^2 = \sum_{i=1}^{A} \vec{r}_i^2 \tag{34}$$

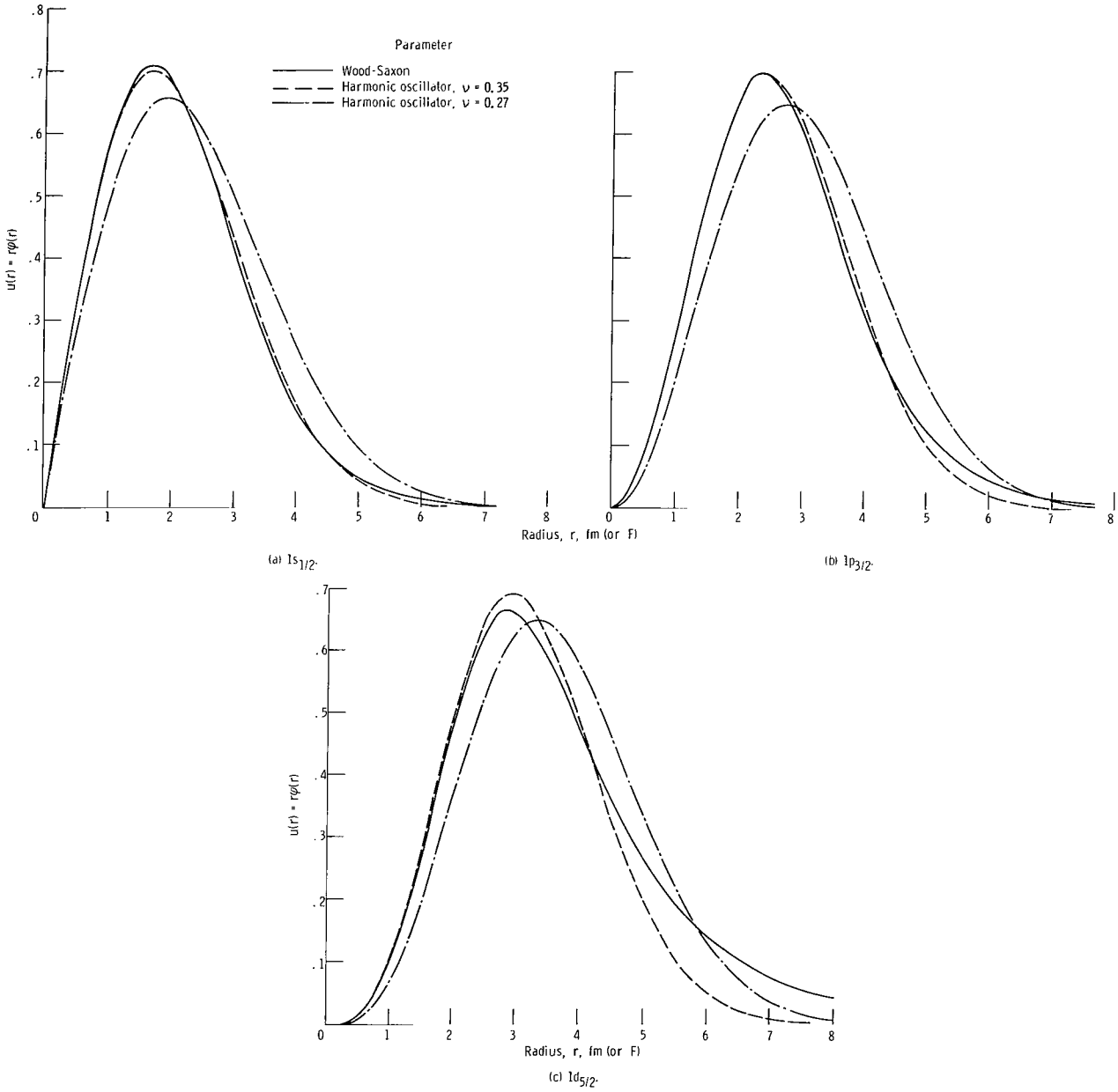
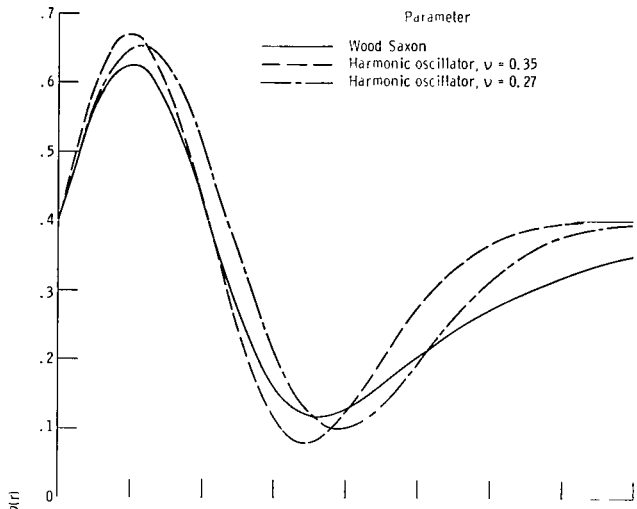
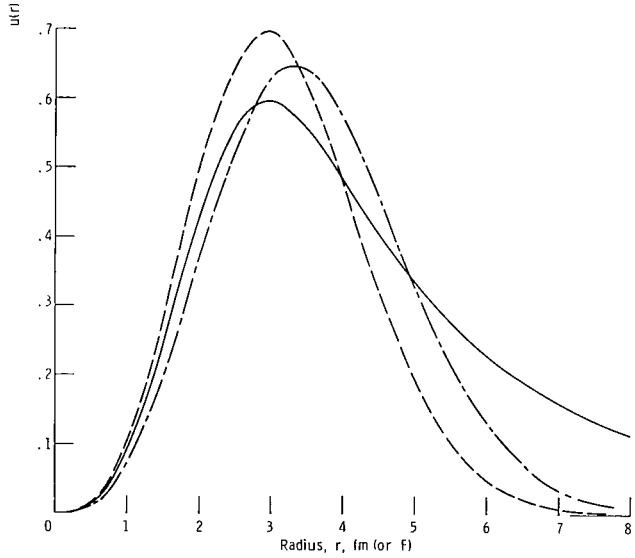


Figure 1. - Single-particle function



(d) $2s_{1/2}$.



(e) $1d_{3/2}$.

Figure 1. - Concluded.

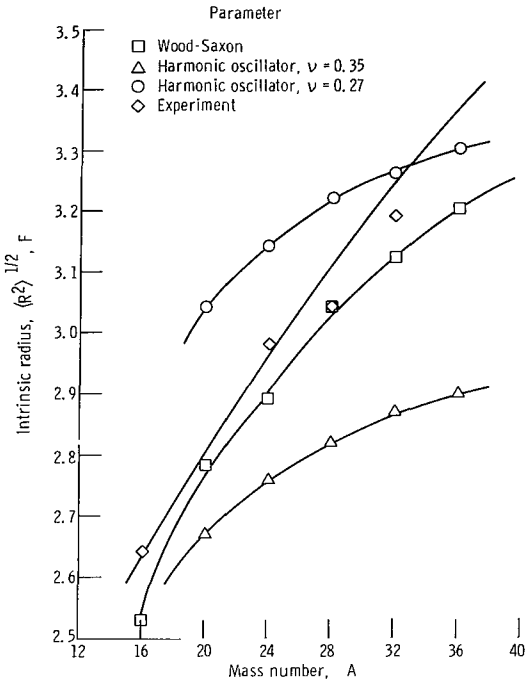
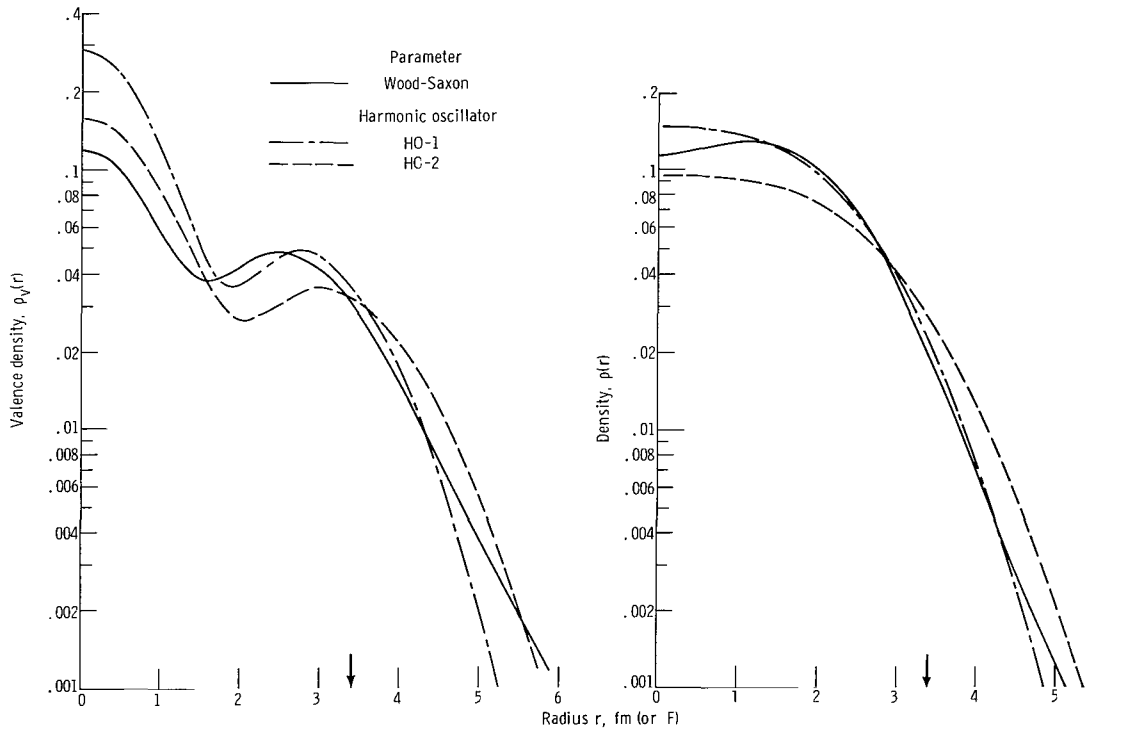


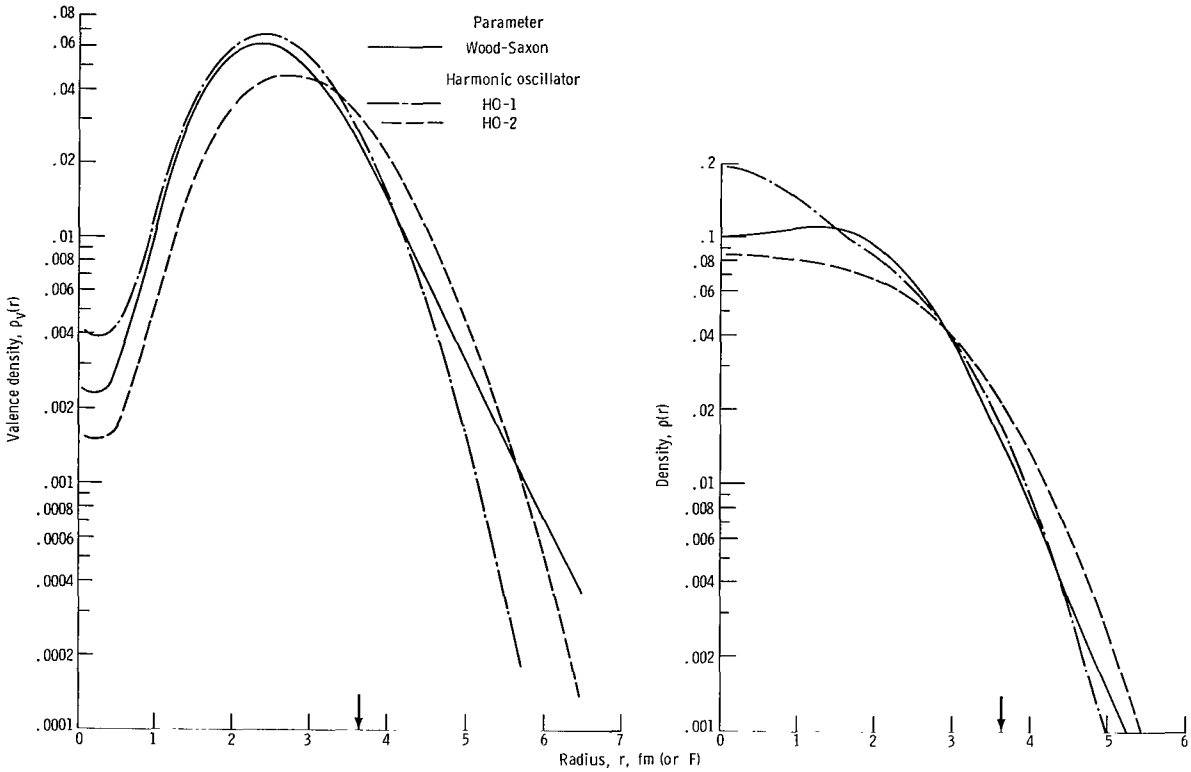
Figure 2. - Intrinsic radius $\langle R^2 \rangle^{1/2}$ against mass number A for the 4n 2s-1d shell nuclei.



(a) Valence density.

(b) Total density.

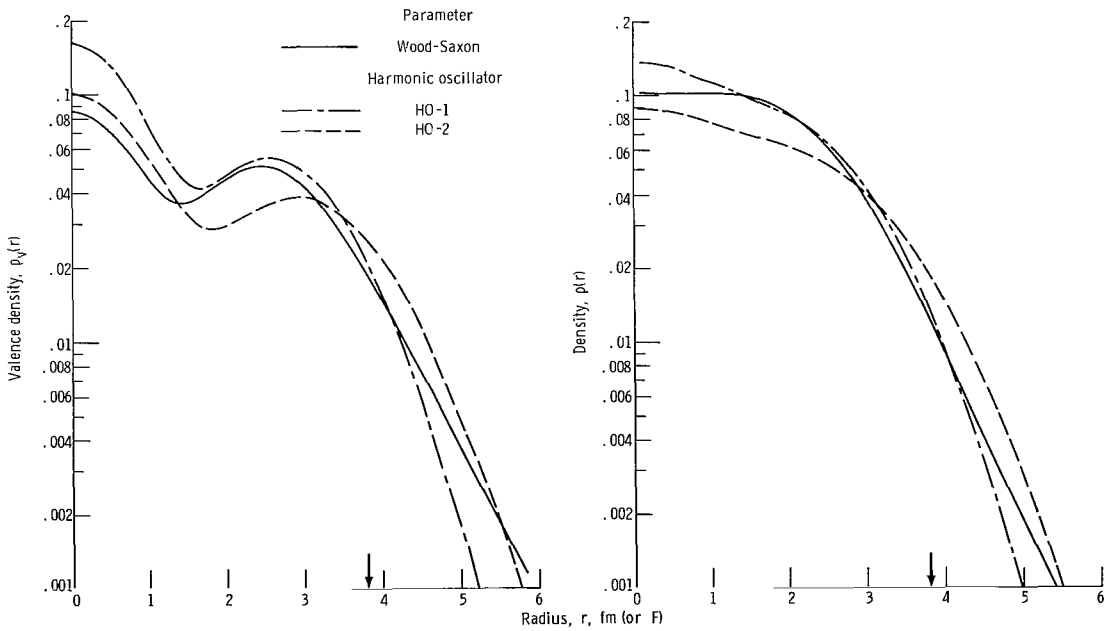
Figure 3. - Densities for neon 20.



(a) Valence density.

(b) Total density.

Figure 4. - Densities for magnesium 24.



(a) Valence density.

(b) Total density.

Figure 5. - Densities for silicon 28.

TABLE II. - ENERGIES AND WAVE FUNCTIONS FOR AXIALLY SYMMETRIC, EVEN-EVEN, 2s-1d SHELL NUCLEI

[Results using a Wood-Saxon basis are in boldface type; light type corresponds to a harmonic oscillator basis with a stated harmonic oscillator parameter ν.]

(a) Harmonic oscillator parameter, $\nu = 0.35\ \mathrm{fm}^{-2}$

Nucleus	Hartree-Fock energy, E_{HF}, MeV	Energy gap, Δ, MeV	Single-particle Hartree-Fock energy, e_λ, MeV	Projection of angular momentum on z-axis, m_λ	Projection of the Hartree-Fock orbits on spherical basis, C_j^λ					
					$1d_{5/2,1/2}$	$1d_{5/2,3/2}$	$1d_{5/2,1/2}$	$2s_{1/2,1/2}$	$1d_{3/2,1/2}$	$1d_{3/2,3/2}$
Ne^{20}	-40.21	10.6	-17.01	1/2	0.6781			-0.6342	-0.3715	
	-35.27	**8.5**	**-14.46**	**1/2**	**.7782**			**-.4943**	**-.3874**	
Mg^{24}	-72.28	4.9	-15.55	3/2		0.9559				-0.2938
	-68.26	**5.0**	**-14.78**	**3/2**		**.9550**				**-.2835**
			-13.83	1/2	0.5414			-0.1080	0.5294	
			-12.78	**1/2**	**.8552**			**-.0997**	**.5086**	
Si^{28}	-132.45	8.2	-21.95	1/2	0.4735			0.8320	-0.2787	
	-116.80	**7.1**	**-18.37**	**5/2**			**1.000**			
			-19.95	5/2			1.000			
			-17.16	**1/2**	**0.6066**			**0.7345**	**-0.3040**	
			-15.86	3/2		0.6440				0.7650
			-13.98	**3/2**		**.6959**				**.7182**
S^{32}	-173.64	5.9	-22.66	1/2	0.4083			0.8830	-0.2315	
	-157.89	**5.0**	**-18.35**	**5/2**			**1.000**			
			-20.24	5/2			1.000			
			-18.11	**1/2**	**0.8167**			**0.4404**	**-0.3730**	
			-18.55	1/2	0.7965			-0.4685	-0.3823	
			-15.14	**1/2**	**-.4162**			**.8972**	**.1481**	
			-16.22	3/2		0.7030				0.7112
			-14.35	**3/2**		**.7889**				**.6145**
Ar^{36}	-238.56	8.1	-25.07	1/2	0.3607			0.9268	-0.1040	
	-209.66	**6.9**	**-21.41**	**5/2**			**1.000**			
			-23.05	5/2			1.000			
			-20.38	**3/2**		**0.9968**				**0.0801**
			-22.27	3/2		0.9969				0.0781
			-19.47	**1/2**	**0.6691**			**0.7419**	**0.0431**	
			-18.94	1/2	0.7411			-0.2172	0.6352	
			-16.16	**1/2**	**.5498**			**-.5332**	**.6429**	
			-17.18	3/2		-0.0781				0.9969
			-14.57	**3/2**		**-.0801**				**.9968**

(b) Harmonic oscillator parameter, $\nu = 0.27\ \mathrm{fm}^{-2}$

Ne^{20}	-34.82	8.2	-14.27	1/2	0.7273			-0.5729	-0.3780	
	-35.27	8.5	-14.46	1/2	.7782			-.4943	-.3874	
Mg^{24}	-65.99	4.8	-14.14	3/2		0.9562				-0.2928
	-68.26	5.0	-14.78	3/2		.9550				-.2835
			-12.52	1/2	0.8333			-0.0809	0.5469	
			-12.78	1/2	.8552			-.0997	.5086	
Si^{28}	-116.41	7.0	-17.34	1/2	0.8290			0.7967	-0.2922	
	-116.80	7.1	-18.37	5/2			1.000			
			-17.55	5/2			1.000			
			-17.16	1/2	0.6066			0.7345	-0.3040	
			-14.07	3/2		0.6682				0.7440
			-13.98	3/2		.6959				.7182
S^{32}	-159.06	5.0	-18.76	1/2	0.5757			0.7598	-0.3020	
	-157.89	5.0	-18.35	5/2			1.000			
			-17.76	5/2			1.000			
			-18.11	1/2	0.8167			0.4404	-0.3730	
			-16.11	1/2	0.6925			-0.6495	-0.3133	
			-15.14	1/2	-.4162			.8972	.1481	
			-14.48	3/2		0.7333				0.6799
			-14.35	3/2		.7889				.6145
Ar^{36}	-211.89	7.1	-20.68	5/2			1.000			
	-209.66	6.9	-21.41	5/2			1.000			
			-20.40	1/2	0.4868			0.8716	-0.0576	
			-20.38	3/2		0.9968				0.0801
			-19.61	3/2		0.9960				0.0895
			-19.47	1/2	0.6691			0.7419	0.0431	
			-16.87	1/2	0.6528			-0.3386	0.6475	
			-16.16	1/2	.5498			-.5332	.6429	
			-15.42	3/2		-0.0895				0.9960
			-14.57	3/2		-.0801				.9968

between HF states Φ. The results, shown in figure 2, differ considerably for the three sets of basis functions, and only the WS results bear a reasonable resemblance to experiment and then only in an average sense. As the mass number increases toward 40, the WS results begin to deviate even more from experiment. The HO results are quite poor in both cases. However, the comparison of all these results with experiment would be much more meaningful if the expectation values were taken with respect to states of good angular momentum. The results are, nonetheless, significant for nuclear matter studies.

Intrinsic Quadrupole Moment

The intrinsic quadrupole moment is defined as the expectation value of the operator

$$Q_o = e\left(\frac{16\pi}{5}\right)^{1/2} \sum_{i=1}^{A} \left[\frac{1 + \tau_3(i)}{2}\right] r_i^2 Y_2^o\left(\Omega_{\vec{r}_i}\right) \tag{35}$$

with respect to HF states Φ. The operator τ_3 is an isospin operator with eigenvalues +1 and -1 for protons and neutrons, respectively; e is the proton charge. In table III the results are given for the intrinsic quadrupole moments. The set HO-2 yields a much better match to the WS than does HO-1. The sign of $\langle Q_o \rangle$ for any particular nucleus does not depend on the choice of basis, and the signs are in agreement with the accepted type of deformation (i.e., prolate or oblate) for these nuclei.

TABLE III. - INTRINSIC QUADRUPOLE MOMENT

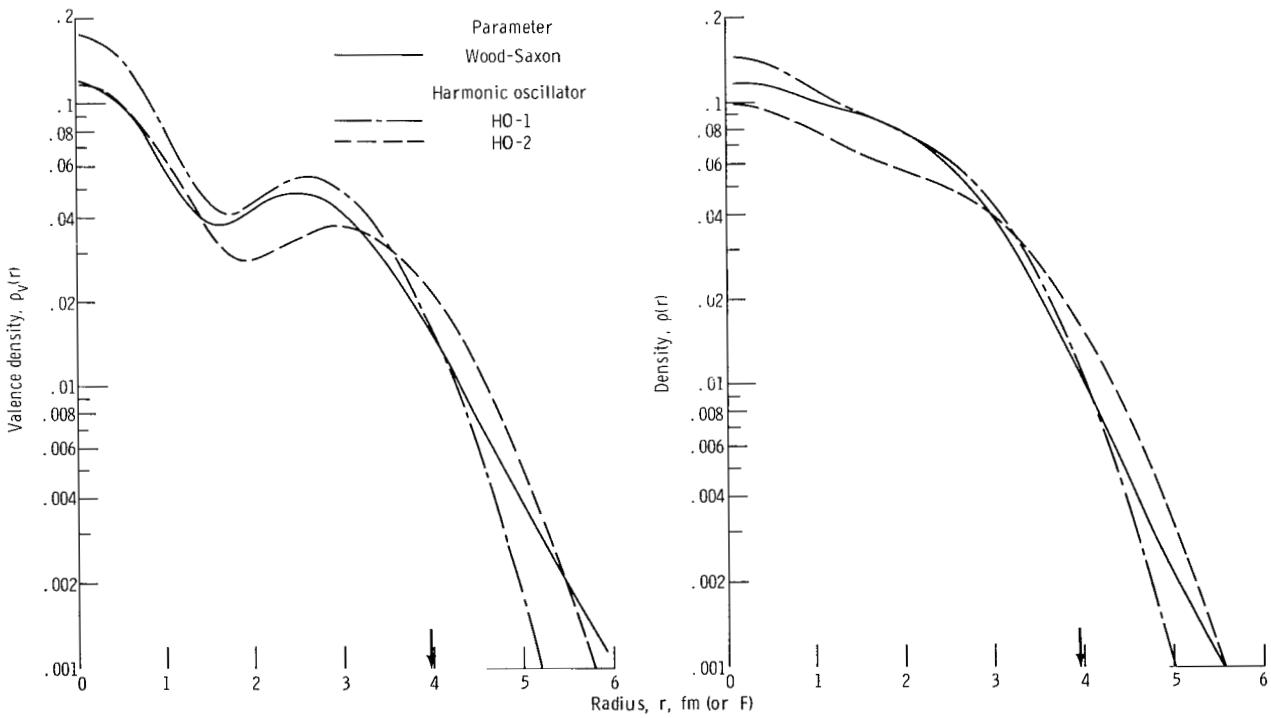
Nucleus	Quadrupole moment, $\langle Q_o \rangle$, e fm^2		
	Harmonic oscillator parameter, ν, fm^{-2}		Wood-Saxon
	$\nu = 0.27$ fm^{-2}	$\nu = 0.35$ fm^{-2}	
Ne^{20}	29.00	22.30	29.24
Mg^{24}	15.80	12.60	14.90
Si^{28}	-42.59	-33.18	-42.51
S^{32}	-12.74	-10.25	-11.74
A^{36}	-25.92	-19.17	-29.65

Nuclear Density

The nuclear density function is defined as the expectation value of

$$\rho = \sum_{i=1}^{A} \delta(\vec{r} - \vec{r}_i) \tag{36}$$

Since the HF calculations of the type presented here test only the extra-core wave functions, two types of density functions are shown for each of the nuclei. The valence density ρ_V is the expectation value of ρ with respect to wave functions which do not specifically include the spherical core functions. The total density $\rho(r)$ does contain the core effects. In figures 3 to 7 the density functions are presented. In each of the figures, parts (a) and (b) refer to valence and total density, respectively. The arrows which appear on each of the figures indicate the position of $1.25\ A^{1/3}$, where A is the mass number. Examination of figures 3 to 7 reveals that both sets of density functions (with the exception of Mg^{24}) show consistent behavior as one goes from Ne^{20} to A^{36}. For the moment the problem of Mg^{24} is set aside, and the general trends for the valence and total densities for the other nuclei are considered.



(a) Valence density.

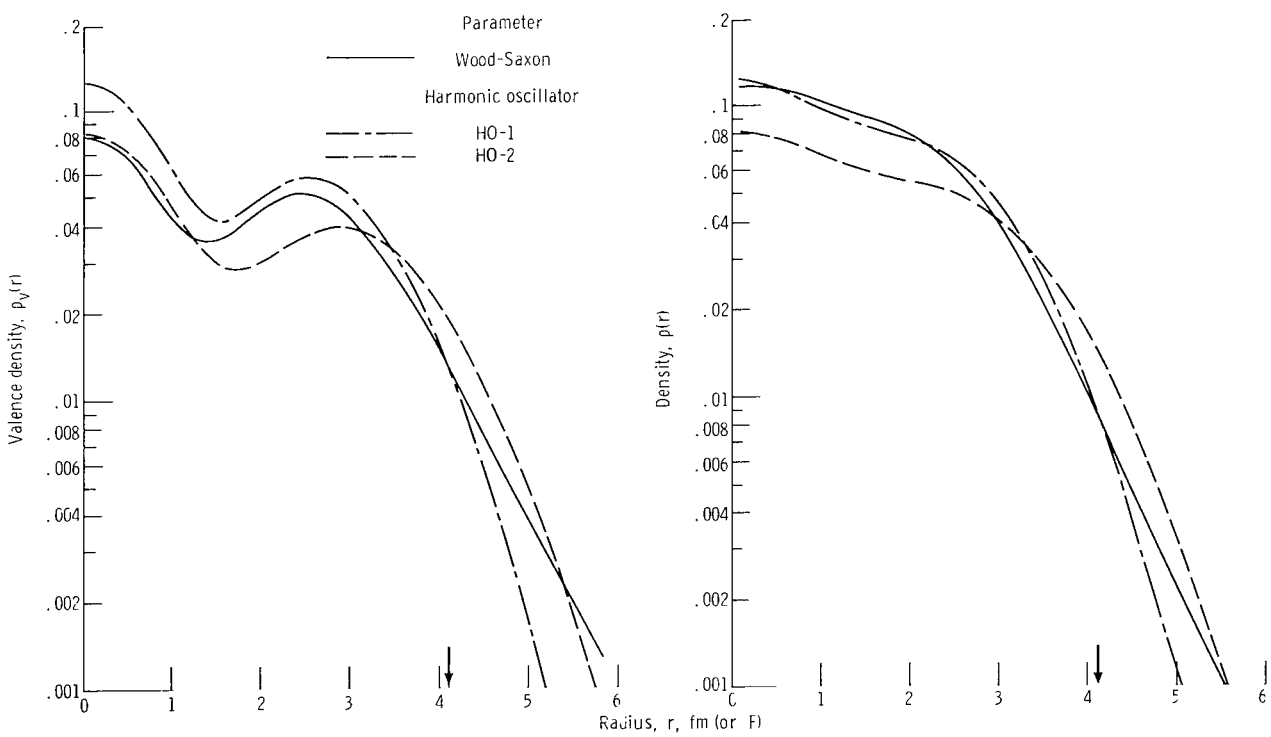
(b) Total density.

Figure 6. - Densities for sulfur 32.

Valence densities. - It is seen from figures 3(a), 5(a), 6(a), and 7(a) that for $0 \leq r \leq 1.5$ the HO-2 ($\nu = 0.27\ \mathrm{fm}^{-2}$) results show better agreement with the WS case than does the HO-1 ($\nu = 0.35\ \mathrm{fm}^{-2}$) result. However, for $1.5 \leq r \leq 4.2$, HO-1 agrees more closely with WS. In the region beyond about 4.2 fm, the HO-1 densities fall off more rapidly than both the WS and HO-2 densities. The three curves focus at about 3.3 fm for all four nuclei.

Total densities. - The total densities are presented in figures 3(b), 5(b), 6(b), and 7(b). For the WS case the flattening near the nuclear center is washed out as A in increases, and all of these total density functions have the same general shape. In the region $1.5 \leq r \leq 4.3$, the HO-1 ($\nu = 0.35\ \mathrm{fm}^{-2}$) results match the WS results quite well, but drop off rapidly beyond $r \approx 4.5$. Beyond $r = 5$ fm it is observed that the HO-2 ($\nu = 0.27\ \mathrm{fm}^{2}$) results agree more closely with WS as might be expected since this is the same region in which the HO-2 wave functions agree most closely with those of the WS potential.

For the case of Mg^{24}, an examination of figure 4(a) perhaps gives an indication as to why Mg^{24} should be treated separately. Certainly the valence density has a peculiar appearance in view of the consistent behavior of the other densities. However, Bar-Touv and Kelson (ref. 8) performed calculations which indicate that Mg^{24} is not axially sym-



(a) Velocity density.

(b) Total densities.

Figure 7. - Densities for argon 36.

metric, so Mg^{24} might be expected to have properties which differ from those of axially symmetric nuclei. Based on the findings of Bar-Touv and Kelson, S^{32} would also be expected to behave similarly, since the same set of calculations indicated that S^{32} is likewise asymmetric. The size of the gaps in the HF spectra (see tables II(a) and (b)) indicate that the assumption of axial symmetry is equally poor for S^{32} and Mg^{24}. That is, since the energy gap between occupied and unoccupied orbits is quite a bit smaller for these nuclei than for the others, a perturbation theory calculation would yield larger effects of axial asymmetry for these nuclei than for the others.

In addition, one of the results of attempting to treat Mg^{24} as axially symmetric is that the coefficient of the $2s_{1/2}$ basis vector turns out to be abnormally small, ~0.10. Consequently, the valence density is drastically reduced at the origin. This does not occur for S^{32}, nor does it occur in an asymmetric treatment (ref. 8) of Mg^{24}.

If asymmetry is assumed, calculations of the energy spectra and other properties of these nuclei, should be more informative than the results just given. However, the previous results do substantiate the belief that Mg^{24} has to be treated differently than the other 2s-1d shell nuclei.

SUMMARY OF RESULTS

The intrinsic energy spectra, radii, and quadrupole moments have been studied for the five even-even nuclei in the 2s-1d shell. The nuclear wave functions were obtained using the HF method. The HF calculations were made using the Wood-Saxon basis functions as well as the more conventional harmonic oscillator basis. It was found that the asymptotic behavior or the WS basis functions could be simulated with harmonic oscillator functions if the oscillator constant were properly chosen. Such oscillator functions were also found to yield the best match to the Woods-Saxon HF spectra, indicating an important dependence on the asymptotic part of the wave function. As expected, Mg^{24} (and to a lesser extent S^{32}) was found to have rather peculiar properties when assumed to be axially symmetric.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, November 25, 1968,
129-02-07-07-22.

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