Hartree-Fock Calculations of Even-Even $N=Z$ Nuclei*

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Hartree-Fock calculations have been performed for the even-even $N=Z$ nuclei from $A=4$ to $A=40$. The calculations use a velocity-dependent interaction which contains two-body spin-orbit and tensor terms, and which was especially derived for use in HF calculations. Effects of truncation are made minimal by using a basis of *Cartesian* harmonic-oscillator wave functions. Nuclear sizes and single-particle energies are in reasonable agreement with experiment; however, total binding energies are much too small. Comparison is made with other recent calculations.

I. INTRODUCTION

THE Hartree-Fock (HF) method has gained increasing popularity as a means of obtaining an understanding of a wide variety of nuclear properties. Since deformed nuclei produce the richest supply of experimental data, it is natural that a large portion of the recent HF literature has concentrated on such calculations.[1] The calculations thus far carried out may be broadly classified according to (1) the type of interaction employed and (2) the size of the model space. The interaction may, in turn, be described as being either (a) a G matrix[2] derived from one of the realistic two-body potentials[3] which account for the free two-nucleon scattering data or (b) an effective potential derived especially for structure calculations. Potentials of the latter type may be further subdivided according to the degree to which they relate to the free two-body data. Thus the potentials of Refs. 4 and 5 may be regarded as being perhaps more fundamental than those of Ref. 6. The model space is normally taken to be a truncated oscillator space in which either the orbitals of (a) all of the particles or (b) only those particles outside closed major shells are varied. Further distinction may be made depending upon the additional restrictions placed upon the variational wave function.

In an effort to understand the validity of some of the approximations made in such computations, I have used a general two-body potential which, although developed especially for use in HF calculations, may yet be described in some sense as having been derived from the free nucleon-nucleon data. Thus the calculation is more fundamental than one which uses a *purely* phenomenological potential, and as such may be viewed as a standard with which to check, for example, the validity of using an effective one-body spin-orbit interaction. Moreover, the present calculation, in addition to varying the orbitals of all particles, utilizes a basis for which the effects of truncation are minimal so that the deformations found are not limited by restrictions on the space of the HF wave function. This latter point is more fully discussed in Sec. II under symmetries of the HF wave function, while the former point is amplified in Sec. III where a brief description is given of the two-body interaction.

The structure of the remainder of the paper is as follows. The method of calculating two-body matrix elements is illustrated in Sec. IV, and the manner of solving the HF equations is discussed in Sec. V. The main results of the calculation are presented in Sec. VI, where energy levels, binding energies, rms radii, and quadrupole moments are given for the even-even $N=Z$ nuclei from $A=4$ to $A=40$. Some concluding remarks are made in Sec. VII.

II. SYMMETRIES OF HF WAVE FUNCTION

Because it is necessary in practice to truncate the basis in which the HF wave function is expanded, the choice of basis is *not* arbitrary. In particular, as we wish to study nuclei which may not be axially symmetric, it will clearly be advantageous to expand the orbitals in a Cartesian oscillator basis

$$|\lambda\rangle=\sum_{n_x n_y n_z \sigma} C_{n_x n_y n_z \sigma}^{\lambda} |n_x\rangle |n_y\rangle |n_z\rangle \chi_\sigma^{1/2}, \quad (1)$$

where

$$\langle x|n_x\rangle=[\pi^{1/2}2^{n_x}n_x!b_x]^{-1/2}H_{n_x}(x/b_x)\exp(-x^2/2b_x^2) \quad (2)$$

and H_{n_x} is the Hermite polynomial given below in

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[1] For an excellent review of the theory as applied to deformed light nuclei, and additional references, see G. Ripka, *Advances in Nuclear Physics* (Plenum Press, Inc., New York, 1968), Vol 1.

[2] T. T. S. Kuo, Nucl. Phys. **A103**, 71 (1967); C. M. Shakin, Y. R. Waghmare, and M. H. Hull, Jr., Phys. Rev. **161**, 1006 (1967); C. W. Wong, Nucl. Phys. **A91**, 399 (1967); A. Kallio and B. D. Day, Phys. Letters **25B**, 72 (1967); D. Grillot and H. McManus, Nucl. Phys. **A113**, 161 (1968); R. J. McCarthy and H. S. Köhler, *ibid.* **A99**, 65 (1967); A. D. MacKellar and R. L. Becker, Phys. Letters **18**, 308 (1965).

[3] K. E. Lassila *et al.*, Phys. Rev. **126**, 881 (1962); T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 383 (1962).

[4] F. Tabakin, Ann. Phys. (N. Y.) **30**, 51 (1964); G. Saunier and J. M. Pearson, Phys. Rev. **160**, 740 (1967); T. F. Hammann and Q. Ho-Kim (unpublished).

[5] C. W. Nestor, K. T. R. Davies, S. J. Krieger, and M. Baranger, Nucl. Phys. **A113**, 14 (1968). The interaction used in the calculations is potential No. 1 of the above reference.

[6] I. Kelson and C. A. Levinson, Phys. Rev. **134**, B269 (1964); J. Bar-Touv and I. Kelson, *ibid.* **138B**, 1035 (1965); A. B. Volkov, Nucl. Phys. **74**, 33 (1965); J. Hayward, *ibid.* **81**, 193 (1966); D. M. Brink and E. Boecker, *ibid.* **A91**, 1 (1967); R. Muthukrishnan, *ibid.* **A93**, 417 (1967). The above represents a partial list of recent HF calculations of *s-d* shell nuclei.

terms of the generating function

$$\exp(-s^2+2s\xi)=\sum_{n=0}^{\infty}\frac{s^n}{n!}H_n(\xi). \tag{3}$$

The advantage of this choice of basis is that the nuclear deformation can be incorporated directly into the basis. That is, by proper choice of the harmonic-oscillator parameters b_x, b_y, b_z we can accelerate the convergence of the calculation with dimensionality. Stated differently, we can produce deformations with a set of basis functions for which $n_x+n_y+n_z\leq 2$ (i.e., the s-d shell in the case $b_x=b_y=b_z$) that a calculation utilizing a basis of spherical oscillator functions could not produce, even if it were to include perhaps the p-f and g shells. The Cartesian basis offers a similar advantage over a cylindrical basis in the study of triaxial nuclei.

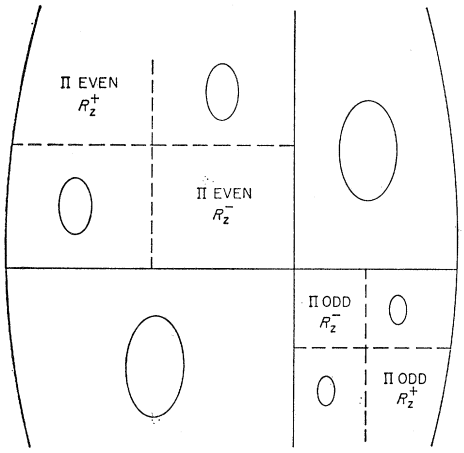


FIG. 1. HF Hamiltonian in the oscillator representation.

In order to minimize the number of two-body matrix elements which must be computed, it is desirable to introduce the expected symmetries of the HF wave function directly into the basis. Although this procedure is extremely attractive from the point of view of making the computation tractable, it is not without its drawbacks. For if we construct the basis in such a manner as to make the occupied orbitals $\{\lambda\}$ invariant under any symmetry operation which commutes with the many-body Hamiltonian H, then the one-body HF Hamiltonian $h(\lambda)$ will also be invariant under the symmetry operation. Thus the symmetry will be propogated from iteration to iteration of the HF equations, with the result that an energetically more favorable solution of lower symmetry may, perhaps, be missed.

We have allowed general ellipsoidal deformation subject to the following additional symmetries. (1) The orbitals are assumed to have good parity. (2) The HF wave function is assumed to be invariant under time reversal. (3) It is invariant under rotations in isospin space. Note that assumptions (2) and (3) together require that each spatial state be fourfold occupied. The validity of assumptions (1) and (2) has been tested

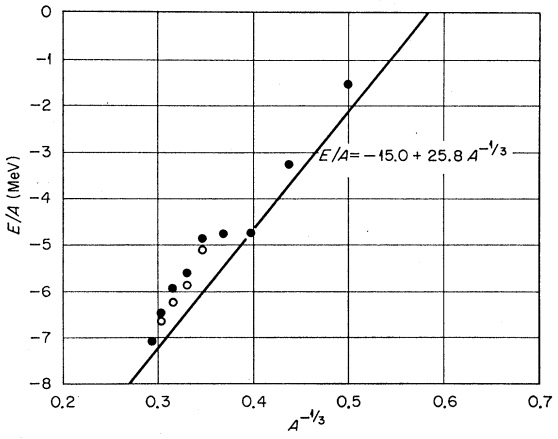


FIG. 2. Binding energy per nucleon. The open circles indicate the approximate energies which would be obtained upon projection, i.e., $E_{J=0}\simeq E_{\rm HF}-\langle J^2\rangle 2I/_{\rm expt}$. The straight line has been drawn as a fit to the spherical nuclei and nuclear matter.

for a number of spherical and deformed nuclei by the MIT group[7] and in all cases, for reasonable interaction strengths, the symmetries have been found valid. For the light nuclei under consideration, neglect of the Coulomb force is a reasonable approximation.

We now demonstrate the computational simplification afforded by the introduction of the above symmetries. Under a rotation of 180° about the z axis, the state $|n_x\rangle|n_y\rangle|n_z\rangle\chi_\sigma^{1/2}$ transforms according to

$$R_z(\pi)|n_x\rangle|n_y\rangle|n_z\rangle\chi_\sigma^{1/2}$$
$$=-i(-)^{\Pi_x+\Pi_y+1/2-\sigma}|n_x\rangle|n_y\rangle|n_z\rangle\chi_\sigma^{1/2}, \tag{4}$$

where $\Pi_i=0$ if n_i is even and $\Pi_i=1$ if n_i is odd $(i=x,y,z)$. The parity of the state will be denoted by Π, $(-)^\Pi=(-)^{\Pi_x+\Pi_y+\Pi_z}$. We construct eigenstates of $R_z(\pi)$ as follows:

$$|\lambda\Pi R_z^+\rangle=\sum_{n_xn_yn_z\sigma}{}' C_{n_xn_yn_z\sigma}^{\lambda}$$
$$\times\tfrac{1}{2}[1+(-)^{\Pi+\Pi_z+1/2-\sigma}]|n_x\rangle|n_y\rangle|n_z\rangle\chi_\sigma^{1/2}, \tag{5a}$$
$$|\lambda\Pi R_z^-\rangle=\sum_{n_xn_yn_z\sigma}{}' C_{n_xn_yn_z\sigma}^{\lambda}$$
$$\times\tfrac{1}{2}[1-(-)^{\Pi+\Pi_z+1/2-\sigma}]|n_x\rangle|n_y\rangle|n_z\rangle\chi_\sigma^{1/2}, \tag{5b}$$

TABLE I. Two-body matrix elements classified by symmetry groups.

Class	Π_α	R_z^α	Π_β	R_z^β
1	Even	R_z^+	Even	R_z^+
2	Even	R_z^+	Even	R_z^-
3	Even	R_z^+	Odd	R_z^-
4	Even	R_z^+	Odd	R_z^+
5	Odd	R_z^-	Odd	R_z^-
6	Odd	R_z^-	Odd	R_z^+
7	Odd	R_z^-	Even	R_z^+
8	Odd	R_z^-	Even	R_z^-

[7] W. H. Bassichis and J. P. Svenne, Phys. Rev. Letters **18**, 80 (1967); M. K. Pal and A. P. Stamp, Phys. Rev. **158**, 924 (1967).

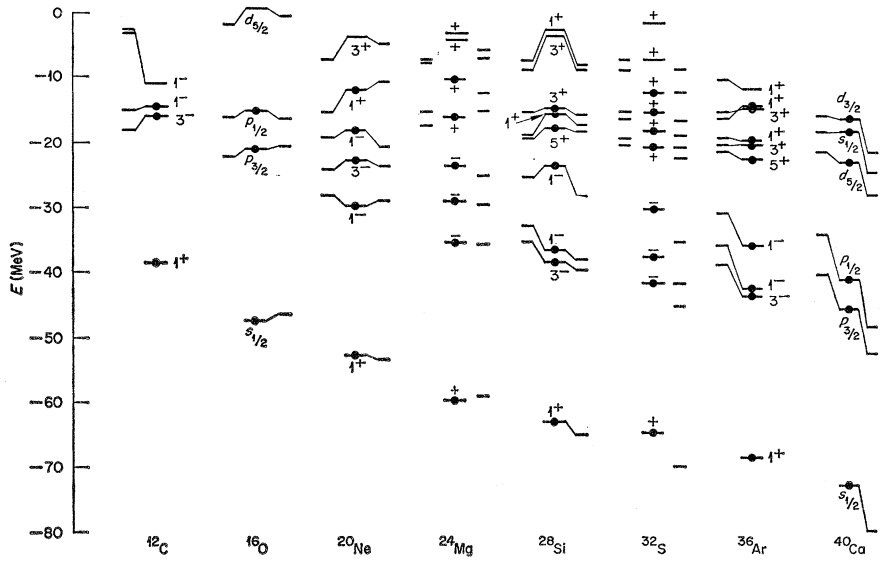


FIG. 3. Single-particle energy levels of the ground-state HF solutions. The central column for each nucleus contains the results of the present calculation. The levels of the axially symmetric nuclei are labeled by the z component of angular momentum k and parity π as $(2k)^{\pi}$; the levels of the triaxial nuclei are labeled by the parity alone. Occupied orbitals are indicated by a dot. The results are to be compared with the calculations of Ripka (Ref. 1) (left column) and Stamp (Ref. 9) (right column).

so that

$$R_z(\pi)\,|\,\lambda\Pi R_z^+\rangle=-i\,|\,\lambda\Pi R_z^+\rangle$$

and

$$R_z(\pi)\,|\,\lambda\Pi R_z^-\rangle=i\,|\,\lambda\Pi R_z^-\rangle. \tag{6}$$

[$|\,\lambda\Pi R_z^+\rangle$ transforms under $R_z(\pi)$ as a particle of spin $+\frac{1}{2}$, while $|\,\lambda\Pi R_z^-\rangle$ transforms as a particle of spin $-\frac{1}{2}$.] The prime indicates that the sum is restricted to those values of n_x, n_y, n_z for which $(-)^{n_x+n_y+n_z}=(-)^{\Pi}$. Since the sums will always be restricted in this manner, the prime will be omitted in future equations.

The states $|\,\lambda\Pi R_z^+\rangle$, $|\,\lambda\Pi R_z^-\rangle$ span our model space and form a natural basis for our wave function. Under a rotation of 180° about the y axis the state $|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_\sigma^{1/2}$ transforms as

$$R_y(\pi)\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_\sigma^{1/2}=(-)^{\pi_x+\pi_z+1/2-\sigma}\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-\sigma}^{1/2}. \tag{7}$$

Thus, according to our assumption of ellipsoidal symmetry, if the state

$$|\,\lambda\Pi R_z^+\rangle=\sum_{n_xn_yn_z}C_{n_xn_yn_z\frac{1}{2}}^{\lambda}\times\tfrac{1}{2}[1+(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{1/2}^{1/2}+C_{n_xn_yn_z-1/2}^{\lambda}\tfrac{1}{2}[1-(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-1/2}^{1/2}$$

is occupied, then the state

$$R_y(\pi)\,|\,\lambda\Pi R_z^+\rangle=|\,\lambda\Pi R_z^-\rangle=(-)^{\Pi}\sum_{n_xn_yn_z}(-)^{\Pi_z}\times\{C_{n_xn_yn_z-1/2}^{\lambda}\tfrac{1}{2}[1-(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{1/2}^{1/2}+C_{n_xn_yn_z\frac{1}{2}}^{\lambda}\tfrac{1}{2}[1+(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-1/2}^{1/2}\}$$

must also be occupied. The states $|\,\lambda\Pi R_z^+\rangle$, $|\,\lambda\Pi R_z^-\rangle$ are thus pairwise occupied. Further we may set $C_{n_xn_yn_z-1/2}^{\lambda}=(-)^{\Pi_x}C_{n_xn_yn_z\frac{1}{2}}^{\lambda}$. Under a rotation of 180° about the x axis we find

$$R_x(\pi)\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_\sigma^{1/2}=-i(-)^{\Pi+\Pi_x}\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-\sigma}^{1/2}, \tag{8}$$

so that

$$R_x(\pi)\,|\,\lambda\Pi R_z^{\pm}\rangle=-i(-)^{\Pi}\,|\,\lambda\Pi R_z^{\mp}\rangle. \tag{9}$$

Since either both of the above states are occupied or both of the states are unoccupied, the HF wave function will be invariant under this rotation. We have thus guaranteed the ellipsoidal symmetry of the HF wave function.

Finally, under time reversal, we have

$$T\alpha\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_\sigma^{1/2}=(-)^{1/2-\sigma}\alpha^*\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-\sigma}^{1/2} \tag{10}$$

and

$$T\,|\,\lambda\Pi R_z^+\rangle=|\,\lambda\Pi R_z^-\rangle=\sum_{n_xn_yn_z}C_{n_xn_yn_z\frac{1}{2}}^{\lambda *}\times\{(-)^{\Pi_x}\tfrac{1}{2}[(-)^{\Pi+\Pi_z}-1]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{1/2}^{1/2}+\tfrac{1}{2}[1+(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-1/2}^{1/2}\}$$

$$=\sum_{n_xn_yn_z}(-)^{\Pi_y}C_{n_xn_yn_z\frac{1}{2}}^{\lambda *}\times\{\tfrac{1}{2}[1-(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{1/2}^{1/2}+(-)^{\Pi_x}\tfrac{1}{2}[1+(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-1/2}^{1/2}\}. \tag{11}$$

The amplitudes $C_{n_xn_yn_z\frac{1}{2}}^{\lambda}$ are thus real if n_y is even and imaginary if n_y is odd. We thus set $C_{n_xn_yn_z\frac{1}{2}}^{\lambda}=(i)^{\Pi_y}a_{n_xn_yn_z}^{\lambda}$. The basis thus takes the final form

$$|\,\lambda\Pi R_z^+\rangle=\sum_{n_xn_yn_z}(i)^{\Pi_y}a_{n_xn_yn_z}^{\lambda}\times\{\tfrac{1}{2}[1+(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{1/2}^{1/2}+(-)^{\Pi_x}\tfrac{1}{2}[1-(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-1/2}^{1/2}\}, \tag{12a}$$

$$|\,\lambda\Pi R_z^-\rangle=T\,|\,\lambda\Pi R_z^+\rangle=\sum_{n_xn_yn_z}(i)^{\Pi_y}a_{n_xn_yn_z}^{\lambda}\times\{\tfrac{1}{2}[1-(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{1/2}^{1/2}+(-)^{\Pi_x}\tfrac{1}{2}[1+(-)^{\Pi+\Pi_z}]\,|\,n_x\rangle\,|\,n_y\rangle\,|\,n_z\rangle\chi_{-1/2}^{1/2}\}. \tag{12b}$$

TABLE II. Nuclear properties. This Table lists the binding energies, rms radii, electric quadrupole moments, and angular momenta for the ground state of the nuclei studied. Experimental radii are taken from Ref. 11.

	B.E. (MeV)	r_{rms} (fm) Theor	Expt	Q_{20} (fm^2)	Q_{22} (fm^2)	$\langle J^2\rangle$
^{4}He	3.30	1.84	1.67	0	0	0
^{8}Be	12.0	2.32		39.0	0	10.5
^{12}C	37.4	2.45	2.42	−17.3	0	8.77
^{16}O	76.3	2.53	2.71	0	0	0
^{20}Ne	95.3	2.77		44.1	0	20.0
^{24}Mg	117.	2.82	2.98	39.3	−7.9	23.6
^{28}Si	157.	3.00	3.04	−63.1	0	29.7
^{32}S	190.	3.12	3.12	−56.1	17.4	27.0
^{36}Ar	233.	3.16		−49.8	0	16.3
^{40}Ca	283.	3.20	3.50	0	0	0

The coefficients $a_{n_x n_y n_z}^{\lambda}$ are real as will be all matrix elements of the HF Hamiltonian between the basis states. The fact that $T\,|\,\lambda\Pi R_z^{\pm}\rangle = \pm\,|\,\lambda\Pi R_z^{\mp}\rangle$ facilitates the evaluation of expectation values of operators, e.g., $\langle \text{HF}\,|\,Q_{20}\,|\,\text{HF}\rangle$ or $\langle \text{HF}\,|\,J^2\,|\,\text{HF}\rangle$.

Due to the above symmetries of the HF wave function, the HF Hamiltonian must necessarily take the form depicted in Fig. 1. Because the orbitals have been assumed to have good parity, the matrix divides into two blocks which operate on the even-parity states and the odd-parity states, respectively. Because of the assumed invariance under time reversal, each of the two blocks further divides into two identical blocks. That the blocks are identical is apparent, for the eigenstates of the blocks, the states R_z^+, R_z^-, are connected by an operator T which commutes with the HF Hamiltonian, and are thus degenerate. Up to this point in our discussion we have suppressed mention of the isospin quantum number. To be specific, the above array may be thought of as operating upon the neutron states. Then, because of the neglect of the Coulomb force, there is an identical array which operates upon the proton states, and each spatial state *is* fourfold occupied, as stated earlier.

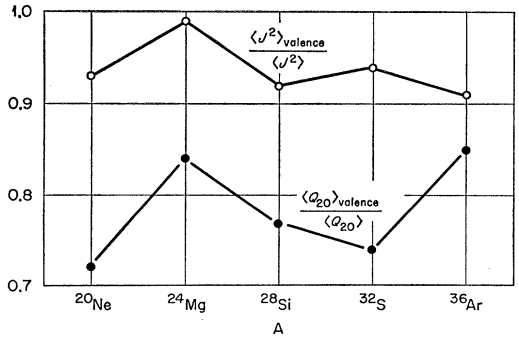


FIG. 4. Contribution of valence particles to the expectation value of the angular momentum and quadrupole moment. The nuclei ^{20}Ne, ^{24}Mg, ^{28}Si are considered as having 4, 8, and 12 valence particles, while ^{32}S and ^{36}Ar are considered as having 4 holes and 8 holes, respectively.

The benefit of the above reduction lies not in the fact that we need only diagonalize two small arrays, e.g., Π even R_z^+ and Π odd R_z^-, but rather that in order to calculate these arrays we need only the two-body matrix elements

$$\langle \mathbf{n}_\alpha \Pi_\alpha R_z^\alpha, \mathbf{n}_\beta \Pi_\beta R_z^\beta SM\,|\,V_T\,|\,\mathbf{n}_\gamma \Pi_\alpha R_z^\alpha, \mathbf{n}_\delta \Pi_\beta R_z^\beta SM'\rangle$$

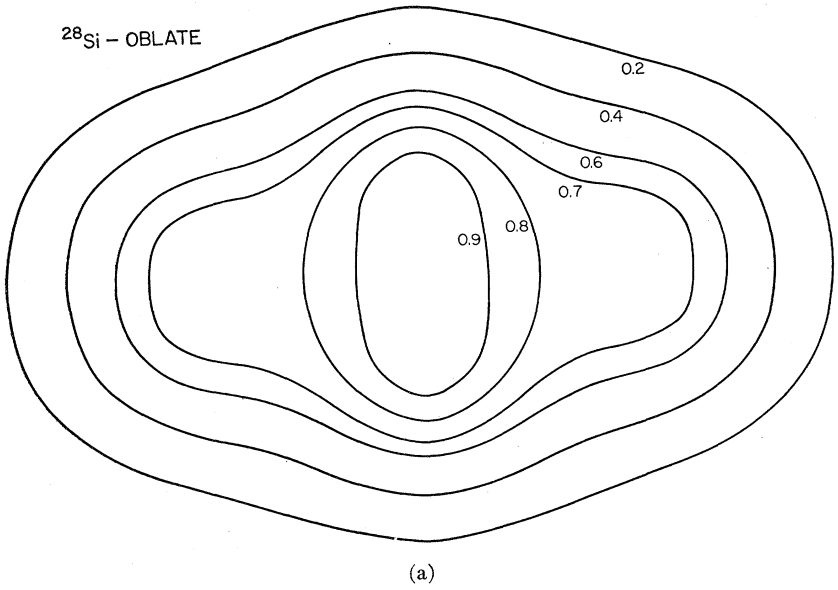
listed in Table I. Further, the matrix elements of class 7 in Table I are clearly identical to those of class 3, while the matrix elements of class 8 are, through time reversal symmetry, equal to those of class 4. Thus, only the matrix elements of classes 1–6 need be computed. This simplification is what makes the computation tractable. For even with the introduction of the symmetries, we must calculate 72 010 (independent) matrix elements for the case $n_x+n_y+n_z\leq 3$.

III. TWO-BODY INTERACTION

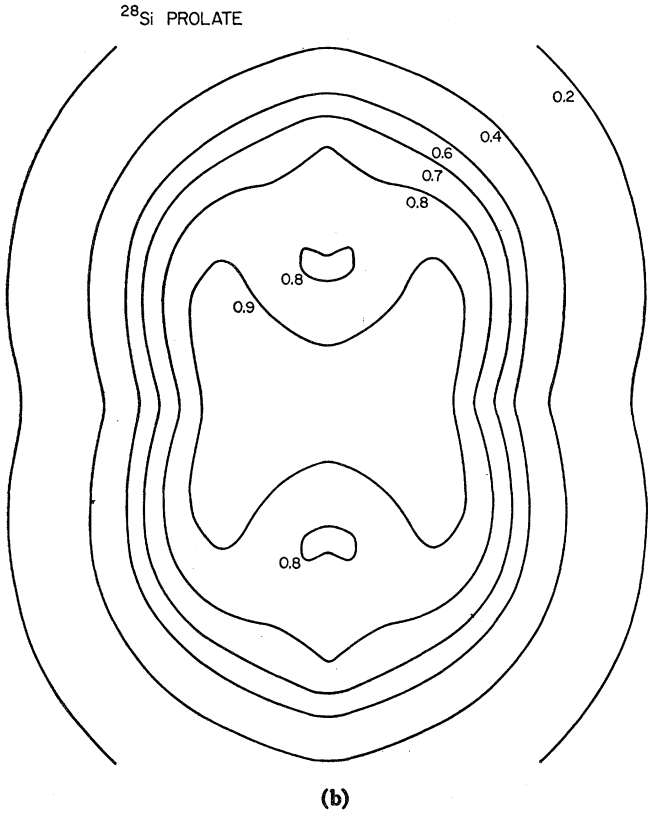
In this work, we use a recently developed velocity-dependent potential which was especially derived for use in HF calculations. The explicit form of the interaction is

$$m/\hbar^2 U_j = V_j^C(r) + (p^2/\hbar^2)\omega_j(r) + \omega_j(r)\,(p^2/\hbar^2) + V_j^T(r)\,S_{12} + V_j^{LS}(r)\mathbf{L}\cdot\mathbf{S}, \quad (13)$$

where m is the nuclear mass and r and p represent the relative coordinate and momentum of the interacting nucleons. $\mathbf{L}$ and $\mathbf{S}$ are the orbital angular-momentum and spin angular-momentum operators and S_{12} is the tensor operator. The index j labels the four spin-parity states of the two-nucleon system, SE, SO, TE, TO. (No spin-orbit interaction has been included in the TE state.) The radial dependence of all terms is Gaussian; however, the tensor term is additionally multiplied by r^2: $V_j^T(r) = -A_j(r^2/2\alpha_j^2)\exp[-(r^2/2\alpha_j^2)]$. With this choice of radial dependence, the interaction is separable in Cartesian coordinates and the computation of two-body matrix elements is thus greatly facilitated.



(a)



(b)

FIG. 5. Cross sections of equidensity surfaces cut by a plane containing the symmetry axis for the oblate and prolate solutions of ^{28}Si. The numerical values refer to the fraction of maximum density: 0.26 and 0.20 fm^{-3}, respectively, for the two solutions.

The potential saturates nuclear matter in the HF approximation at $k_F = 1.38$ fm^{-1} with an energy $E_0 = -15$ MeV. The second-order Goldstone correction to the energy, calculated in the effective-mass approximation, is -3.2 MeV. The low-energy scattering produced by the potential can be summarized as follows. The accepted values for the scattering lengths and effective ranges are fitted to within 5%, and the deuteron binding energy and quadrupole moment are fitted to within 10%. However, the percentage d state in the deuteron is calculated to be 2% which is much lower than the accepted value of approximately 6%.

TABLE III. Single-particle binding energies in MeV. With the exception of the $d_{5/2}$ level which, in the deformed nuclei is almost pure $d_{5/2}{}^{5/2}$, the energies of the deformed nuclei are labeled by $(2k^{\pi})$; e.g., 3^- indicates a state of negative parity with z component of angular momentum $\frac{3}{2}$. The experimental results are taken from Ref. 15. For ^{40}Ca the italicized energies represent neutron levels; all other experimental energies are for protons. For the deformed nuclei we have suggested a comparison with the state(s) which contain a significant amount of the single-particle strength; no attempt has been made to compute the center of gravity of the levels.

	^{16}O		^{20}Ne		^{28}Si		^{36}Ar		^{40}Ca		
	Theor	Expt	Theor	Expt	Theor	Expt	Theor	Expt	Theor		Expt
$1s_{1/2}$	47	44							**73**		**≈75**
$1p_{3/2}$	21	19	(3^-) 23	19, 18	(3^-) 38	36			**46**		
											≈32
$1p_{1/2}$	15	12	(1^-) 30, 18	12	(1^-) 36, 23	28			41		
$1d_{5/2}$					17	**17**	22	20	23	*22*	16
$2s_{1/2}$					(1^+) 16, 2	13			18	*18*	8
$1d_{3/2}$									16	*16*	8

Complete details concerning this potential are given in Nestor *et al.*[5] For calculations of the closed-shell nuclei with this potential, see Tarbutton and Davies.[8]

IV. CALCULATION OF TWO-BODY MATRIX ELEMENTS

We must calculate the antisymmetrized matrix elements

$$\langle \mathbf{n}_1\mathbf{n}_2M \mid U_{ST} \mid \mathbf{n}_1'\mathbf{n}_2'M'\rangle_A = \langle \mathbf{n}_1\mathbf{n}_2M \mid U_{ST} \mid \mathbf{n}_1'\mathbf{n}_2'M'\rangle - (-)^{S+T}\langle \mathbf{n}_1\mathbf{n}_2M \mid U_{ST} \mid \mathbf{n}_2'\mathbf{n}_1'M'\rangle, \quad (14)$$

where $\mathbf{n}$ denotes the principal quantum numbers, $\mathbf{n}=(n_x, n_y, n_z)$, and $\langle \mathbf{n}_1\mathbf{n}_2M \mid U_{ST} \mid \mathbf{n}_1'\mathbf{n}_2'M'\rangle$ is the matrix element for distinguishable particles, and describes the scattering event in which particles $1'$ and $2'$ in the harmonic-oscillator orbitals $\mathbf{n}_1'\mathbf{n}_2'$, respectively, with total spin S, z component of spin M', and isospin T, are scattered into the orbitals $\mathbf{n}_1$, $\mathbf{n}_2$ with z component of spin M. (The two-body potential conserves total spin and isospin.)

We introduce the Talmi transformation to relative and c.m. coordinates

$$|\mathbf{n}_1\mathbf{n}_2\rangle = \sum_{\mathbf{nN}} \langle \mathbf{nN} \mid \mathbf{n}_1\mathbf{n}_2\rangle \mid \mathbf{nN}\rangle. \quad (15)$$

TABLE IV. Comparison of nuclear deformations. The second column contains the results of the present work, while the third column contains the (major-shell mixing) results of Ripka (Ref. 1).

Nucleus	$\langle 2z^2-x^2-y^2\rangle/\langle x^2+y^2+z^2\rangle$	
^{12}C	−0.48	−0.47
^{20}Ne	0.57	0.59
^{28}Si oblate	−0.50	−0.49
^{28}Si prolate	0.58	0.75
^{32}S prolate	0.33	0.35
^{36}A	−0.28	−0.24

[8] R. M. Tarbutton and K. T. R. Davies, Nucl. Phys. **A120**, 1 (1968).

For Cartesian oscillator functions, the transformation is particularly simple for the transformation bracket immediately factors into three one-dimensional brackets with

$$\langle n_iN_i \mid n_{1i}n_{2i}\rangle = (-)^{n_i}/2^{[(n_i+N_i)/2]}\left(\frac{n_{1i}!n_{2i}!}{n_i!N_i!}\right)^{1/2} \times \sum_m (-)^m \binom{n_i}{m}\binom{N_i}{n_{2i}-m}\delta_{n_{1i}+n_{2i},n_i+N_i}. \quad (16)$$

[$i=x$, y, or z and

$$\binom{a}{b}$$

is the standard binomial coefficient.] Computation of the matrix element has thus been reduced to evaluation of the sum

$$\langle \mathbf{n}_1\mathbf{n}_2M \mid U_{ST} \mid \mathbf{n}_1'\mathbf{n}_2'M'\rangle = \sum_{\mathbf{nNn}'} \langle \mathbf{n}_1\mathbf{n}_2 \mid \mathbf{nN}\rangle\langle \mathbf{n}'\mathbf{N} \mid \mathbf{n}_1'\mathbf{n}_2'\rangle \times [1-(-)^{n_x'+n_y'+n_z'+S+T}]\langle \mathbf{n}(\mathbf{N})M \mid U_{ST} \mid \mathbf{n}'(\mathbf{N})M'\rangle. \quad (17)$$

Note that the above sum is, in fact, over only three variables. For if, e.g., we fix $\mathbf{N}$, then $\mathbf{n}$ and $\mathbf{n}'$ are determined by the requirement that the transformation bracket be nonvanishing. The matrix element in relative coordinates may be calculated very easily as we illustrate in the case of the central forces.

For velocity-independent central forces,

$$\langle \mathbf{n}(\mathbf{N})M \mid U_{ST} \mid \mathbf{n}'(\mathbf{N})M'\rangle = -A_{ST}\langle n_x \mid\mid \exp(-x^2/2\alpha_{ST}{}^2) \mid\mid n_x'\rangle \times \langle n_y \mid\mid \exp(-y^2/2\alpha_{ST}{}^2) \mid\mid n_y'\rangle \times \langle n_z \mid\mid \exp(-z^2/2\alpha_{ST}{}^2) \mid\mid n_z'\rangle \quad (18)$$

TABLE V. Wave functions for the oblate and prolate solutions of ^{28}Si.

	^{28}Si (Oblate) $b_x=b_y=1.877$ $b_z=1.514$				^{28}Si (Prolate) $b_x=b_y=1.684$ $b_z=2.017$			
Even-parity states								
	$(2k)^\pi$	1^+	5^+	1^+	3^+	1^+	1^+	3^+	1^+
$n_xn_yn_z\sigma$	ϵ	−63.0	−17.4	−15.2	−14.6	−59.7	−19.9	−15.0	−10.4
000↑		0.999	0.000	0.036	0.000	0.999	0.004	0.000	0.011
i110↑		0.000	0.707	0.000	−0.685	0.000	0.000	0.074	0.000
200↑		−0.027	0.500	0.695	0.485	−0.035	−0.014	−0.052	−0.080
020↑		−0.027	−0.500	0.695	−0.485	−0.035	−0.014	0.052	−0.080
002↑		−0.028	0.000	−0.092	0.000	0.000	0.955	0.000	−0.030
−101↓		0.005	0.000	−0.110	−0.174	−0.012	0.209	0.703	0.671
i011↓		−0.005	0.000	0.110	−0.174	0.012	−0.209	0.703	−0.671
Odd-parity states									
	$(2k)^\pi$	3^-	1^-	1^-		1^-	3^-	1^-	
$n_xn_yn_z\sigma$	ϵ	−38.3	−36.4	−23.3		−39.8	−30.3	−26.0	
001↑		0.000	0.157	0.988		0.994	0.000	−0.109	
−100↓		0.707	0.698	−0.111		0.077	0.707	0.703	
i010↓		0.707	−0.698	0.111		−0.077	0.707	−0.703	

with

$$\langle n_x \| \exp(-x^2/2\alpha_{ST}^2) \| n_x' \rangle = \int_{-\infty}^{\infty} dx u_{n_x}(x) \times \exp(-x^2/\alpha_{ST}^2) u_{n_x'}(x) = \tfrac{1}{2}[1+(-)^{n_x+n_x'}] \times \left(\frac{n_x! n_x'!}{2^{n_x+n_x'}}\right)^{1/2} \frac{(-)^{(n_x-n_x')/2}}{(1+\alpha_{ST}^2/b_x^2)^{1/2(n_x+n_x'+1)}} \times \sum_l \frac{(2\alpha_{ST}^2/b_x^2)^l}{[\tfrac{1}{2}(n_x-l)]![\tfrac{1}{2}(n_x'-l)]!l!}. \quad (19)$$

The index l runs from the minimum of n_x, n_x' down in units of two to zero or one. The velocity-dependent term requires, in addition, the evaluation of the reduced matrix element

$$\langle n_x \| p_x^2 \exp(-x^2/2\alpha_{ST}^2) + \exp(-x^2/2\alpha_{ST}^2) p_x^2 \| n_x' \rangle = (1/b_x^2)[n_x+n_x'+1-(\alpha_{ST}^3/2b_x^2)(\partial/\partial\alpha_{ST})] \times \langle n_x \| \exp(-x^2/2\alpha_{ST}^2) \| n_x' \rangle, \quad (20)$$

where in deriving the above we have made use of the fact that $|n_x\rangle$ is a solution of the harmonic-oscillator equation in one dimension.

Since we have parametrized the radial form of the interaction so that it separates in Cartesian coordinates, the noncentral portions of the potential may be evaluated as readily. Details are given in the Appendix. Thus the computation of any given matrix element proceeds very rapidly. This obviously is an essential condition for the present calculation since it is necessary to compute such a vast number of matrix elements.

V. SOLUTION OF HF EQUATIONS

Because we are dealing with nonspherical nuclei, we expect to find a multiplicity of solutions to the HF equations, corresponding to various deformations. There are two main methods which one may use to explore the various solutions. The first method utilizes the fact that the HF equations are to be solved by an iterative technique. We pick an initial density matrix, evaluate the HF potential Γ, diagonalize the HF Hamiltonian $h=T+\Gamma$, recompute Γ with a new density matrix determined by filling the orbitals of lowest energy obtained in the diagonalization of h, and iterate until the sequence converges. Thus, all possible solutions should be found by simply exhausting all of the ways in which one can choose the initial density matrix. An alternative method is to force the nucleus to change deformation by placing it in an external (quadrupole) field. If the external field is large compared to the self-consistent nuclear field, then the nuclear shape will be determined by the external field and the nucleus can be driven (discontinuously, due to shell structure) from one solution to another. This latter method is particularly useful in gaining insight into the nature of excited states of collective nature, since it enables one to map the energy surface in the vicinity of a true solution. For the present, we restrict ourselves to a discussion of the solution at the true minima and adopt the first method outlined above. The Cartesian basis, as it turns out, is once again a rather natural one in that it is fairly easy to intuitively pick initial density matrices, which then converge to the desired results.

We then proceed by choosing a density matrix

$$\rho_{\mathrm{n}_2\sigma_2;\mathrm{n}_1\sigma_1}=\sum_{\lambda\ \text{occupied}} a_{\mathrm{n}_2}^{\lambda} a_{\mathrm{n}_1}^{\lambda}, \tag{21}$$

compute the HF potential

$$\Gamma_{\mathrm{n}\tau;\mathrm{n}'\sigma'}=\sum_{\mathrm{n}_1\sigma_1\mathrm{n}_2\sigma_2 TS} \tfrac{1}{2}(2T+1)C_{\sigma\sigma_1 M}^{\frac{1}{2}\frac{1}{2}S} C_{\sigma'\sigma_2 M'}^{\frac{1}{2}\frac{1}{2}S} \times\langle \mathrm{n}\mathrm{n}_1 M \mid U_{ST} \mid \mathrm{n}'\mathrm{n}_2 M'\rangle_A \rho_{\mathrm{n}_2\sigma_2;\mathrm{n}_1\sigma_1}, \tag{22}$$

add to it the kinetic energy matrix

$$t_{\mathrm{n}\sigma;\mathrm{n}'\sigma'}=\langle \mathrm{n}\sigma \mid \mathbf{p}^2/2m \mid \mathrm{n}'\sigma'\rangle$$

to form the HF Hamiltonian, and iterate as described above.

VI. RESULTS

The results presented here use a basis of oscillator functions with $n_x+n_y+n_z\leq 2$. No significant improvement is obtained by including the set of functions with $n_x+n_y+n_z=3$. Thus, for example, if we minimize the ground-state energy of ^{28}Si using the lower dimensionality and then, without further change of the oscillator parameters, increase the basis, we find less than a 1% change in the total binding energy, single-particle energies, and nuclear size and shape.

Our results are in general agreement with the results of Ripka[1] and of Stamp.[9] Thus, we find that the nuclei ^{20}Ne, ^{28}Si, and ^{36}Ar are axially symmetric with ^{20}Ne prolate, and ^{28}Si and ^{36}Ar oblate, while ^{24}Mg and ^{32}S are triaxial. Although the shapes agree with the general arguments put forth by Banerjee *et al.*,[10] two of the nuclei ^{28}Si and ^{32}S possess solutions of different symmetry which in each case lie less than 4 MeV above the lower-energy solution.

Table II[11] lists some of the results of the study. In addition to total binding energies and rms radii, we give the (intrinsic) electric quadrupole moments Q_{20}, Q_{22} as defined by

$$Q_{2m}=\sum_{\text{protons}} (16\pi/5)^{1/2}\langle r^2 Y_{2m}\rangle, \tag{23}$$

and also the expectation value of the angular momentum $\langle J^2\rangle$. As may be seen, the nuclear sizes are in reasonable agreement with experiment. Using the adiabatic approximation,[12] we have compared the intrinsic quadrupole moment of ^{20}Ne with that obtained in a shell-model calculation[13] and find our result of 44 fm^2 in reasonable agreement with the extracted value of 49 fm^2. The shell-model calculation used an effective charge $\frac{1}{2}e$.

The binding energy per particle is plotted versus $A^{-1/3}$ in Fig. 2. Note that the deformed nuclei lie above the straight line which is drawn as a fit to the spherical nuclei ^{16}O and ^{40}Ca and nuclear matter. Thus, higher-order correlations omitted in HF appear to be of more importance for the open-shell nuclei.[14]

In Fig. 3, we compare the single-particle energies of the ground-state HF solutions with those of Ripka[1] and Stamp.[9] Where comparison is possible, there is qualitative and, in most cases, semiquantitative agreement. The levels of the axially symmetric nuclei are compared with experiment in Table III,[15] where the agreement is again reasonable.

Further comparison with the results of Ripka[1] is made in Table IV where it may be seen that, with the exception of the excited (prolate) state solution of ^{28}Si, there is rather remarkable agreement on nuclear shapes. The contribution of the valence particles to the electric quadrupole moment and to $\langle J^2\rangle$ is plotted in Fig. 4, where it is seen that the core contribution to Q_{20} is somewhat less than the $\sim$30% found in calculations using a basis of spherical oscillator functions.[1] In order to obtain a more graphic representation of the varied equilibrium shapes, we have plotted in Figs. 5(a) and 5(b) equidensity surfaces in the plane containing the symmetry axis for the oblate and prolate solutions of ^{28}Si. The corresponding wave functions are given in Table V. The results for the prolate solution, $B.E.=153$ MeV, $r_{\mathrm{rms}}=3.06$ fm, $Q_{20}=76.1$ fm^2, and $\langle J^2\rangle=28.1$, may be compared with the corresponding numbers for the oblate solution which are given in Table II. The near identity of the rms radii for the two solutions does not in itself provide a very valid test of the volume conservation hypothesis, for the value of this parameter is very heavily influenced by the nuclear *surface*. In an effort to obtain a more meaningful comparison, we have calculated the volumes of the oblate, prolate, and spherical states of ^{28}Si as defined by

$$V=\int \mathrm{d}^3 r\,\Theta[\rho(\mathbf{r})-0.2\rho_{\max}], \tag{24}$$

i.e., the volume in which the density is no less than 20% of the maximum density. We find that the volumes defined in this manner differ by less than 10%. A more accurate determination of this volume might reduce the variance to 5%.

VII. CONCLUSIONS

In looking over various efforts, nearly all nuclear calculations yield rather similar results for the energy levels and equilibrium shapes of the light nuclei. Thus,

[9] A. P. Stamp, Nucl. Phys. **A105**, 627 (1967).
[10] M. K. Banerjee, C. A. Levinson, and G. J. Stephenson, Jr., Phys. Rev. **178**, 1709 (1969).
[11] R. Hofstadter and H. R. Collard, *Landolt-Börnstein* (Springer-Verlag, Berlin, 1967).
[12] A. Bohr and B. Mottelson, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **27**, 16 (1953).
[13] I am indebted to J. B. McGrory for a discussion of this recent result of the Oak Ridge shell-model group.
[14] S. J. Krieger, Phys. Rev. Letters **22**, 97 (1969).
[15] G. J. Wagner, Bull. Am. Phys. Soc. **14**, 85 (1969); L. R. B. Elton and A. Swift, Nucl. Phys. **A94**, 52 (1967).

although we still place a high priority on the development of an interaction which can be used throughout the Periodic Table, it is clear that the more phenomenological potentials developed for a specific region of the table, here specifically the *s-d* shell nuclei, will yield completely consistent results in that region. In particular, the effective one-body spin-orbit interaction appears to be an adequate approximation for the calculation of light nuclei.

We have further shown that a basis of Cartesian oscillator functions is extremely efficient in minimizing the effects of truncation. Although this advantage will only become more pronounced when one attempts to calculate the large deformations in the heavy fissionable nuclei, it must unfortunately be weighed against the huge number of two-body matrix elements which is required in this representation.

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APPENDIX: MATRIX ELEMENTS OF NONCENTRAL PORTION OF INTERACTION

For the spin-orbit interaction, we must compute

$$\langle \mathbf{n}_1\mathbf{n}_2 SM \mid V_j \mathbf{L}\cdot\mathbf{S} \mid \mathbf{n}_1'\mathbf{n}_2' SM'\rangle = \sum \langle \mathbf{n}_1\mathbf{n}_2 \mid \mathbf{n}\mathbf{N}\rangle \langle \mathbf{n}'\mathbf{N} \mid \mathbf{n}_1'\mathbf{n}_2'\rangle [1-(-)^{n'+S+T}] \times \langle \mathbf{n} \mid\mid \mathbf{r}\times\mathbf{p}[-A_j \exp(-r^2/2\alpha_j^2)] \mid\mid \mathbf{n}'\rangle \times \langle SM \mid \tfrac{1}{2}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2) \mid SM'\rangle. \quad (25)$$

The spin matrix element is given by

$$\langle SM \mid \tfrac{1}{2}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2) \mid SM'\rangle = \delta_{S1}[(1/\sqrt{2})(\delta_{M',M-1}+\delta_{M',M+1})\hat{x} - (i/\sqrt{2})(\delta_{M',M-1}-\delta_{M',M+1})\hat{y} + M\delta_{MM'}\hat{z}], \quad (26)$$

and the x component of the reduced matrix element in coordinate space by

$$\hat{x}\cdot\langle \mathbf{n} \mid\mid \mathbf{r}\times\mathbf{p} \exp(-r^2/2\alpha_j^2) \mid\mid \mathbf{n}'\rangle = \langle n_x \mid\mid \exp(-x^2/2\alpha_j^2) \mid\mid n_x'\rangle \{\tfrac{1}{2}i[(b_y/b_z)-(b_z/b_y)] \times \langle n_y \mid\mid (y/b_y)\exp(-y^2/2\alpha_j^2) \mid\mid n_y'\rangle \times \langle n_z \mid\mid (z/b_z)\exp(-z^2/2\alpha_j^2) \mid\mid n_z'\rangle + i[(n_y+1)^{1/2}(b_z/b_y)\langle n_z \mid\mid (z/b_z)\exp(-z^2/2\alpha_j^2) \mid\mid n_z'\rangle \times \langle n_y+1 \mid\mid \exp(-y^2/2\alpha_j^2) \mid\mid n_y'\rangle - (n_z+1)^{1/2}(b_y/b_z)\langle n_y \mid\mid (y/b_y)\exp(-y^2/2\alpha_j^2) \mid\mid n_y'\rangle \times \langle n_z+1 \mid\mid \exp(-z^2/2\alpha_j^2) \mid\mid n_z'\rangle]\}. \quad (27)$$

The reduced matrix element

$$\langle n_y \mid\mid y\exp(-y^2/2\alpha_j^2) \mid\mid n_y'\rangle = \left(\frac{n_y!n_y'!}{2^{n_y+n_y'-1}}\right)^{1/2} \frac{(-)^{\frac{1}{2}(n_y-n_y'-1)}(\alpha_j^3/b_y^2)}{[1+(\alpha_j^2/b_y^2)]^{\frac{1}{2}(n_y+n_y'+2)}} \times \left\{\sum_l \frac{(2\alpha_j^2/b_y^2)^l}{[\frac{1}{2}(n_y-1-l)]![(n_y'-l)]!l!}\left[1-\frac{n_y'-l}{l+1}\left(\frac{\alpha_j}{b_y}\right)^2\right] -\tfrac{1}{2}[1-(-)^{n_y}]\{[\tfrac{1}{2}(n_y)]![\tfrac{1}{2}(n_y'-1)]!\}^{-1}\right\}. \quad (28)$$

The matrix element as given above is for $n_y'<n_y$ and n_y', n_y of opposite parity. The sum over l runs from n_y' down in units of 2 to 0 or 1. For the tensor interaction, we must compute

$$\langle \mathbf{n}_1\mathbf{n}_2 SM \mid V_j S_{12} \mid \mathbf{n}_1'\mathbf{n}_2' SM'\rangle_A = \sum_{\mathbf{n}\mathbf{N}\mathbf{n}'} \langle \mathbf{n}_1\mathbf{n}_2 \mid \mathbf{n}\mathbf{N}\rangle \langle \mathbf{n}'\mathbf{N} \mid \mathbf{n}_1'\mathbf{n}_2'\rangle \times [1-(-)^{n'+S+T}](24\pi/5)^{1/2} \times \langle \mathbf{n} \mid\mid Y_2(r)[-A_j(r^2/2\alpha_j^2)\exp(-r^2/2\alpha_j^2)] \mid\mid \mathbf{n}'\rangle \cdot \langle SM \mid T_2(\sigma_1,\sigma_2) \mid SM'\rangle. \quad (29)$$

The spin-matrix element is given by[16]

$$\langle SM \mid T_{2q}(\boldsymbol{\sigma}_1,\boldsymbol{\sigma}_2) \mid SM'\rangle = \delta_{S1}(20/3)^{1/2} C_{M'qM}^{121}. \quad (30)$$

The reduced matrix element in coordinate space requires, in addition to the elements which we have displayed previously,

$$\langle n_y \mid\mid y^2\exp(-y^2/2\alpha_j^2) \mid\mid n_y'\rangle = \alpha_j^3(\partial/\partial\alpha_j)\langle n_y \mid\mid \exp(-y^2/2\alpha_j^2) \mid\mid n_y'\rangle. \quad (31)$$

Note that the matrix elements are given between HOWF's which do *not* include the additional phase factors included in the definition of our basis states.

[16] D. M. Brink and G. R. Satchler, *Angular Momentum* (Clarendon Press, Oxford, 1968). It is amusing to note that, with the exception of the spin-$\frac{1}{2}$ Clebsch-Gordan coefficients which appeared in the expression for the HF potential, this is the only vector coupling coefficient to appear in the entire calculation.