the stripping calculations fit the data fairly well and it is expected that stripping is the main process for the (α,t) reaction, contributions from other processes such as knockon or heavy-particle stripping (as suggested by the backward peaking in the angular distribution to the 4.97-MeV level) remain open questions. These contributions can be properly studied only when finite-range calculations are available for these processes.

The large cross section to the 4.25-MeV level is perhaps the most interesting result of this work. It should stimulate more refined theoretical calculations for the wave functions of Ne^{20} and other neighboring nuclei. The calculation of the contribution from higher configurations other than the $1d$, $2s$ shell can help to pin down the mechanism of the reaction. In particular, once these contributions of the higher shells are known, they will shed light on the role of "indirect" processes such as inelastic excitations in this reaction.

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Hartree-Fock Calculations with Realistic Hard-Core Potential

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The effective matrix elements of the two-nucleon Yale potential have been used in doing Hartree-Fock (HF) calculations in $N=Z$ even nuclei ($8\leq A\leq 40$). The ground-state energy and single-particle energies and wave functions have been calculated as a function of two deformation parameters. The calculated equilibrium shapes and binding energy per nucleon are found to be reasonably good. The difficulties in the HF formalism due to the state dependence on the reaction matrix have been discussed, and methods suggested for doing a fully self-consistent calculation of the reaction matrix elements and the Hartree-Fock energy and states.

I. INTRODUCTION

ATOMIC nuclei are known to exhibit both single-particle and collective properties. An interplay of the two modes is also observed. Systems possessing similar kinds of motion have been encountered elsewhere in physics (e.g., the electron gas exhibiting collective plasma oscillation), and adequately treated in a unified theoretical frame. Similar unification has been achieved in the nuclear-structure theory in recent years.

Considerable time elapsed between the development of the unified outlook in nuclear-structure theory, and the initial proposal of the structural models: the nuclear shell model and the collective model. These models were empirical in spirit and helped to explain and systematize numerous experimental data on single-particle and collective nuclear properties, respectively. The initial understanding was handicapped by the dilemma of the successful application of the shell model on the one hand, and the strong two-nucleon interactions (having a hard-core in some states), derived from an analysis of two-body binding and scattering data, on the other. In more detailed spectroscopic calculations,[1] using the shell model, various brands of smooth well-behaved exchange-dependent potentials that are much weaker than the observed two-nucleon potentials, have been successfully used as the residual interaction between the valence nucleons. In a somewhat different approach,[2] the two-body matrix elements themselves have been treated as parameters to be determined by fitting the closed-shell plus two-nucleon nuclei, and then the spectra of neighboring nuclei calculated in terms of these matrix elements. Although such work rests heavily on the assumption of simple shell-model configurations for the nuclei under consideration, it is fairly successful in many regions of the Periodic Table. What is important here is that the effective two-body matrix elements found in such work, once again, are of fairly reasonable magnitude and bear no relation at all to the matrix elements of the "actual" two-nucleon potential (which are infinitely large because of the hard core) between shell-model states.

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[1] J. P. Elliott and A. M. Lane, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 39, p. 241. This review article describes many spectroscopic calculations using smooth residual interactions.

[2] I. Talmi and I. Unna, Ann. Rev. Nucl. Sci. **10**, 353 (1960); I. Talmi, Rev. Mod. Phys. **34**, 704 (1962).

The proper understanding came with the development of the theory of nuclear matter by Brueckner and collaborators,[3] Bethe and Goldstone,[4] and Gomes, Walecka, and Weisskopf.[5] It has been shown that the Pauli exclusion principle makes a fundamental difference between the correlated motion of a pair of nucleons when they are left to themselves, and when they are embedded in a many-nucleon medium. In the former case the strong interaction gives rise to a strongly correlated wave function exhibiting large phase shifts at large separation distance. On the other hand, in the second case the Pauli principle prevents a given pair of nucleons to scatter to states occupied by other nucleons in the Fermi sea; the correlation built up as a result of scattering to very high momentum states is confined only to a very small separation distance ($\sim$1 F), after which the wave function quickly "heals up" (a term used in Ref. 5) to the free-nucleon wave function without any phase shift. It has further been shown[6] that the effect of third- or higher-order clustering of nucleons in nuclei is also very small.

Thus, one should allow every pair of nucleons to interact as many times as possible, obeying the Pauli exclusion principle, and calculate the resultant energy of the pair, and then sum such pair energies for all the pairs in the nucleus. That will give the ground-state energy of the nucleus. The pair energy that results from multiple scattering of a pair through the actual potential may be interpreted as the value of an effective-potential operator for the given pair state. This operator is usually known as the reaction operator, and denoted variously by the symbols t, G, or K. We shall always use the symbol t in this paper.

The quick healing up of the correlated pair wave function (ψ) to the uncorrelated wave function (ϕ) accounts for the success of an independent-particle model of the nucleus. However, the above discussion emphasizes that the effect of the actual short-range correlation present in the pair wave function has to be taken into account by using the effective potential t along with the uncorrelated wave functions. The correlated wave function has a zero, where the hard-core potential v has its singularity, and as a result the matrix elements of the effective potential between uncorrelated states $(\phi_m|t|\phi_n)$, which is identically equal to $(\phi_m|v|\psi_n)$, are well-defined finite quantities.

Associated with the calculation of the t matrix is the concept of two sets of states: (1) the low-lying states make the first set and they comprise two types: (a) states that are filled up in the ground state, and (b) those which lie above, but near the top of the occupied levels. The importance of the type-b states is that the residual interaction mixes them with the type-a states and depletes the sharp Fermi sea (i.e., the ground state with levels up to a certain maximum occupied by particles). In a nucleus with an unfilled major shell, the states belonging to set (1) determine the ground-state and low-energy properties of the nucleus. Mixing among them may cause the so-called BCS pairing phenomenon in the ground state, or an intrinsic deformation to a nonspherical shape, etc. (2) The second set of states lie very much above the low-lying set; these are the states to which a pair of nucleons in the nucleus predominantly scatter as a result of the strong two-nucleon interaction having the hard core. The excited intermediate states that enter in the calculation of the correlated pair wave function (and, hence the t matrix) belong to this set. We shall arbitrarily use the following nomenclatures to denote the different kinds of states: "occupied" states (set 1, type a), "unoccupied" states (set 1, type b), "excited intermediate" states (set 2).

The effect of the excited intermediate states are taken into account in calculating the t-matrix elements, which should then be used with the occupied and unoccupied states (i.e., set 1) to calculate the ground-state and low-energy properties of the nucleus. The next step in this unified structure theory will be to *calculate* the single-particle states belonging to set 1, self-consistently, using the two-body t-matrix elements and the Hartree-Fock (HF) formalism. The effect of the residual interactions can then be taken into account by a random-phase-approximation (RPA) treatment[7] to yield collective vibrational properties. On the other hand, if the HF treatment yields a deformed ground state, then states of good angular momentum can be projected out[8] which will yield the collective rotational properties.

The self-consistent theory, however, is more complicated in principle than the above discussion would suggest. The effective two-body matrix elements (i.e., the t matrix) used in such a calculation depend on the energy spectrum and wave functions that result out of the self-consistent calculation itself. This double self-consistency requirement is very cumbrous to satisfy in practice. To bypass this difficulty, it is customary[9,10] to ignore the self-consistency requirement in the calculation of the t matrix. In this work we have

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[4] H. A. Bethe and J. Goldstone, Proc. Roy. Soc. (London) **A238**, 551 (1957).

[5] L. C. Gomes, J. D. Walecka, and V. F. Weisskopf, Ann. Phys. (N. Y.) **3**, 241 (1958).

[6] H. A. Bethe, Phys. Rev. **138**, B804 (1965); S. A. Moszkowski, *ibid.* **140**, B283 (1965).

[7] R. A. Ferrell, Phys. Rev. **107**, 1631 (1957); P. W. Anderson, *ibid.* **112**, 1900 (1958); S. Fallieros, thesis, University of Maryland, 1959 (unpublished); Maryland Technical Report No. 128, 1959 (unpublished); M. Baranger, Phys. Rev. **120**, 957 (1960).

[8] R. E. Peierls and J. Yoccoz, Proc. Phys. Soc. (London) **A70**, 381 (1957); W. H. Bassichis, B. Giraud, and G. Ripka, Phys. Rev. Letters **15**, 980 (1965).

[9] T. T. S. Kuo and G. E. Brown, Phys. Letters, **18**, 54 (1965); Nucl. Phys. **85**, 40 (1966); R. L. Becker and A. D. McKeller, Phys. Letters **21**, 201 (1966).

[10] C. Shakin, Y. R. Waghmare, and M. H. Hull (to be published).

adopted the same simplifying assumption, and have done self-consistent calculations with the t-matrix elements of the Yale potential,[11] determined once for all by Shakin[10] using harmonic-oscillator wave functions and energies. We have, however, discussed at length ways to improve upon this approximation, and reach the ultimate goal of achieving double self-consistency. This has been done mainly with a view to indicate our future program of work, which will be reported elsewhere.

The present work is one of the few initial attempts at using a realistic hard-core potential in HF calculations. Shakin and Waghmare[10] have used their effective matrix elements in doing HF calculations on closed-shell spherical nuclei: O^{16}, Ca^{40}, and Zr^{90}. In the present work we lay the main emphasis on non-closed-shell nuclei, and exploring the nature of their deformation. To the knowledge of the present authors, no HF calculations have yet been done with the Hamada-Johnston hard-core potential,[12] for which the effective matrix elements have already been evaluated by Kuo and Brown,[9] and by MacKeller and Becker.[9]

Another realistic potential, which does not have a hard core, was set up by Tabakin[13] with the specific intention of applying it to HF calculations. His potential is separable nonlocal, and is smooth well behaved, and as such, very easy in its application. It has been used by Kerman, Svenne, and Villars[14] for closed-shell nuclei: O^{16} and Ca^{40}. The inadequate binding energy, obtained in this work, has recently been improved upon by Pal, Svenne, and Kerman,[15] by including the second-order terms. Self-consistent calculations, including the second-order effects of the Tabakin potential, are now being carried out for non-closed-shell nuclei by Bassichis and Kerman.[16]

HF calculations have also been done by Baranger *et al.*[17] using a simple separable nonlocal potential, and a smooth velocity-dependent potential. These authors adopt the view that, in choosing a good two-body effective potential for HF work, one should be guided more by its ability to produce rapid convergence in a many-body theory, rather than an extremely good fit to the detailed two-body data. The potentials they have used were chosen to satisfy the above criterion.

In earlier HF work by Levinson, Kelson, and others,[18] a smooth well-behaved Yukawa potential with Rosenfeld exchange mixture was very widely used. These authors further confined their self-consistent calculations to the nucleons in the last unfilled major shell, and used experimental numbers to simulate the properties of the core. The importance of their calculations lay in demonstrating that a HF calculation is practicable in nuclei, and such calculations lead to extremely interesting results on the energy gap in single-particle energy spectrum, the shape and the moment of inertia of the nucleus.

In their exploration of the shape of nuclei, Bar-Touv and Kelson[18] used various shapes of the single-particle density to start the HF calculation, and then compared the ground-state energies obtained in the different cases. In this work we have followed a more systematic way, using the method of Lagrange multipliers, to follow the energy surface as a function of two deformation parameters, β and γ, the former giving the amount of spheroidal deformation and the latter the departure from spheroidal to ellipsoidal shape. This method was suggested by Kerman,[19] and has been used by Bassichis and Kerman[16] in doing deformed HF calculations restricted to spheroidal symmetry.

We have done the calculations for all even-even ($N=Z$) nuclei in the range Be^8 to Ca^{40}. All the harmonic-oscillator wave functions up to the $2s$-$1d$ major shell were used as basis in the HF diagonalization. In Sec. II we present the general HF formalism and its specialization to the hard-core potential. This section also contains a scheme of future calculations in which the effective two-body matrix elements themselves are made self-consistent with respect to the HF states and energies. Section III gives many details of the actual HF computations, namely the choice of the initial density satisfying general symmetry properties, its subsequent changes through the Lagrange multiplier method, exploration of the energy-surface versus the deformation parameters, etc. Numerical results are described and presented with the help of tables and curves in Sec. IV. Section V discusses some of the limitations of the present calculations, and points out unexplored areas into which future work of the self-consistent type could expand itself.

II. HARTREE-FOCK FORMALISM FOR A HARD-CORE POTENTIAL

A. General Formalism

The nuclear Hamiltonian for a system of A nucleons is given by

$$H=\sum_{i=1}^{A} T_i+\sum_{i<j}^{A} v_{ij} \tag{1a}$$

or its equivalent second-quantized form:

$$H=\sum_{\alpha,\beta}\langle\alpha|T|\beta\rangle c_\alpha^\dagger c_\beta+\tfrac{1}{2}\sum_{\alpha,\beta,\gamma,\delta}\langle\alpha\beta|v|\gamma\delta\rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma. \tag{1b}$$

[11] K. E. Lassila, M. H. Hull, Jr., H. M. Ruppel, F. A. McDonald, and G. Breit, Phys. Rev. **126**, 881 (1962).
[12] T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 382 (1962).
[13] F. Tabakin, Ann. Phys. (N. Y.) **30**, 51 (1964).
[14] A. K. Kerman, J. P. Svenne, and F. M. Villars, Phys. Rev. **147**, 710 (1966).
[15] M. K. Pal, J. P. Svenne, and A. K. Kerman (to be published).
[16] W. H. Bassichis and A. K. Kerman (to be published).
[17] K. T. R. Davies, S. J. Krieger, and M. Baranger, Nucl. Phys. **84**, 545 (1966).
[18] I. Kelson and C. A. Levinson, Phys. Rev. **134**, B269 (1964); J. Bar-Touv and I. Kelson, *ibid.* **138**, B1035 (1965).
[19] A. K. Kerman, Ann. Phys. (N. Y.) **12**, 300 (1961).

T and v are, respectively, the kinetic- and potential-energy operators; α, β, etc., represent a complete set of single-particle basis states for which $c_\alpha^\dagger$, c_α are, respectively, the creation and destruction operators. In the Hartree-Fock method one assumes a ground-state wave function in a determinantal form in which certain single-particle states l, m, $n\cdots$, etc., are occupied. These wave functions are first expressed in terms of the single-particle basis states as follows:

$$|l\rangle=\sum_\alpha x_\alpha{}^l|\alpha\rangle, \tag{2a}$$

subject to the normalization condition

$$\sum_\alpha |x_\alpha{}^l|^2=1. \tag{2b}$$

Then, the coefficients $x_\alpha{}^l$ are treated as variational parameters for the minimization of the expectation value $\langle H\rangle$ of the Hamiltonian in the determinantal ground state. We have

$$\begin{aligned}\langle H\rangle&\equiv\sum_{l=1}^A\langle l|T|l\rangle+\sum_{l<m}^A\langle lm|v|lm\rangle_a\\&=\sum_{l=1}^A\sum_{\alpha\beta}x_\alpha{}^{l*}x_\beta{}^l\langle\alpha|T|\beta\rangle\\&\quad+\sum_{l<m}^A\sum_{\alpha\beta\gamma\delta}x_\alpha{}^{l*}x_\gamma{}^l x_\beta{}^{m*}x_\delta{}^m\langle\alpha\beta|v|\gamma\delta\rangle_a\end{aligned} \tag{3}$$

and the minimization of this expression yields the equation

$$\sum_\beta\langle\alpha|T|\beta\rangle x_\beta{}^l+\sum_\beta\langle\alpha|V|\beta\rangle x_\beta{}^l=\epsilon_l x_\alpha{}^l; \tag{4}$$

ϵ_l is a Lagrange multiplier that multiplies Eq. (2b) in the process of variation, and the single-particle HF potential V is defined by

$$\langle\alpha|V|\beta\rangle=\sum_{\gamma,\delta}\langle\alpha\gamma|v|\beta\delta\rangle_a\rho_{\delta\gamma}, \tag{5a}$$

where

$$\rho_{\delta\gamma}=\sum_{m=1}^A x_\delta{}^m x_\gamma{}^{m*}\equiv\sum_{m=1}^A\langle\delta|m\rangle\langle m|\gamma\rangle. \tag{5b}$$

The operator

$$\rho=\sum_{m=1}^A|m\rangle\langle m|$$

is clearly the single-particle density operator, and $\rho_{\delta\gamma}$ are its matrix elements with respect to the single-particle basis states. The label a on the two-body matrix elements in Eqs. (3) and (5a) denote matrix elements for antisymmetric two-body states (i.e., direct minus exchange).

The program, to be carried out, for the minimization of ground-state energy, thus reduces to the solution of the single-particle eigenvalue eigenfunction, Eq. (4). Since the operator V is defined in terms of the eigenvector x, a question of self-consistency is involved here. This is usually achieved by repeated diagonalization of $T+V$, starting with a guess for ρ and then recalculating ρ, and hence V, from the eigenvector at each iteration.

B. Specialization to a Hard-Core Potential—Double Self-Consistency

The description of the HF method given here is fairly standard, and the same equations may be obtained in many different ways (see, e.g., Baranger).[20] These derivations, however, do not hold for a realistic two-nucleon potential that possesses a hard core, because the two-body matrix elements for the basis states become infinite. As a result, although (1a) still represents the Hamiltonian to be solved, the second-quantized version (1b) in terms of the matrix elements of v for the basis states becomes meaningless.

Fortunately, however, for a hard-core potential, the Brueckner-Goldstone many-body theory[3–5] gives rise to an expression for the ground-state energy, *in the lowest order*, resembling Eq. (3), except for the fact that v is now replaced by the reaction operator t. The latter was described physically in the introductory section, and an exact mathematical definition will soon follow. One can, as before, minimize the new expression,

$$\langle H\rangle=\sum_{l=1}^A\langle l|T|l\rangle+\sum_{l<m}^A\langle lm|t|lm\rangle_a, \tag{6}$$

with respect to the coefficients $x_\alpha{}^l$ of (2a), subject to the restriction (2b), and obtain Eq. (4) to be diagonalized. The definition of V, however, now changes to

$$\langle\alpha|V|\beta\rangle=\sum_{\gamma,\delta}\langle\alpha\gamma|t|\beta\delta\rangle_a\rho_{\delta\gamma} \tag{7}$$

with the same definition (5b) for ρ.

There is, however, some minor formal difficulties which will be pointed out later on. We first define t in terms of v:

$$t=v-v(Q/e)t. \tag{8}$$

Here, Q is the operator that takes care of the Pauli exclusion principle, i.e., it restricts the intermediate states of the pair of nucleons, originally belonging to the occupied set l, m, $n\cdots$, etc., to states outside the set. The energy denominator e is the difference between the energies of the pair of nucleons in their excited intermediate state and their initial state. The single-particle energies, to be used in the energy denominator should be the same as determined in the HF calculation. Thus, as mentioned in the introduction, there is a

[20] M. Baranger, *Theory of Finite Nuclei, 1962 Cargèse Lectures on Theoretical Physics*, edited by M. Lévy (W. A. Benjamin, Inc., New York, 1963).

question of double self-consistency involved here. Not only must the single-particle wave functions and energies determined in the HF diagonalization be self-consistent, they should also reproduce self-consistently the matrix elements of t. This now brings us to the formal difficulties mentioned above. The minimization of Eq. (6) should have given rise to additional terms due to the implicit dependence of t, through Q/e, on the single-particle states. We shall arbitrarily ignore such terms and assume that the HF equation is still *approximately* good for the minimization of energy.

From the definition of the Pauli operator Q given above, it is clear that the intermediate states could, strictly speaking, belong to the "unoccupied" set as well as the "excited intermediate" set (nomenclatures defined in Sec. I). In practice, however, it is necessary to exclude the former set also from the intermediate states. This set of states, being very close to the "occupied" set of states, cannot be important as far as the scattering of a pair of nucleons by the strong short-range part of the force is concerned. On the other hand, the high-lying excited intermediate states are very important as far as such scattering is concerned; the effective potential that results, being a weak, and rather long-ranged (see Scott and Moszkowski[21]) potential can mix the low-lying unoccupied states very well with the occupied ones. The unoccupied levels play a major role in this type of mixing, and an extremely unimportant role in the formation of the effective potential itself. Therefore, to avoid double-counting of their contribution, it is very important that they be omitted as intermediate states in calculating t, and considered only in the subsequent diagonalization process.

C. Simplifying Assumptions for t-Matrix Elements

In the case of infinite nuclear matter the self-consistent calculation becomes easier because the single-particle wave functions are always plane waves; only the energies need be determined self-consistently. Kuo and Brown[9] have introduced an approximation in the finite-nucleus calculation in analogy with the above-mentioned simplification for the case of nuclear matter. They argue that the single-particle wave functions for finite nuclei very nearly resemble harmonic-oscillator wave functions and hence one may forget about making them self-consistent, and achieve self-consistency only in the energy denominator. In the actual calculations they have gone a step further, and used the harmonic-oscillator energies or a reference spectrum. Once this second approximation is introduced, there is no requirement of self-consistency at all in their calculation of the t-matrix elements with harmonic-oscillator states. These numbers can then be looked upon as the matrix elements, in oscillator basis, of the effective potential, and used in Eq. (7) to carry out HF calculations in a straightforward manner. This is the viewpoint adopted in the present work. We have used the t-matrix elements in oscillator basis for the Yale potential (calculated by Shakin[10] in a somewhat different way) in the HF calculation without bothering about the self-consistency of the t-matrix elements themselves. A few comments on Shakin's method of derivation of the matrix elements will be given in the Appendix.

D. Improved Methods of Calculating Self-Consistent t Matrix

Although not very relevant to the numerical results presented in this paper, we would like to indicate here several ways of improving upon the above-mentioned viewpoint.

(1) The first is to adopt the view that the oscillator wave functions are being used merely as basis wave functions in the t-matrix calculations. Then, for each set of initial energy $\epsilon_m+\epsilon_n$ (obtained from the HF spectrum and treated as a parameter), one can calculate the full set of matrix elements of t in the oscillator basis. As discussed by Bethe, Brandow, and Petschek,[22] this t matrix is Hermitian, and is dependent on the parameter $(\epsilon_m+\epsilon_n)$. But then one immediately runs into formal troubles in the definition (7) of V. These matrix elements of V depend on the choice of the initial occupied pair state. All one can hope for, under the circumstances, is that this dependence is not strong and, hence, can be averaged out to give a fairly meaningful definition of the matrix elements of the v in the chosen basis.

(2) A slight variant of the procedure, which is much easier to carry out, will be to use an average quantity Δ for the energies $(\epsilon_m+\epsilon_n)$ in the calculation of the t matrix. The HF spectrum may be used as a guide in choosing a value for Δ. It is expected that such a choice will make the difference $(Q/e-1/e_m)$ very small. e_m is the energy denominator calculated with Δ.

(3) The most rigorous procedure is to calculate the t matrix at each iteration of the HF equations, in the representation of the contemporary HF single-particle states. With such matrix elements, one can define the matrix elements of V in the same representation as follows:

$$(r|V|s)=\tfrac{1}{2}\sum_m [(rm|t|sm)+(sm|t|rm)], \qquad (9)$$

where $|r)$ and $|s)$ can be both occupied and unoccupied single-particle states, and the summation on m runs over the occupied states only. To make V Hermitian, we now need the explicit symmetrization on the right-hand side.

In the definition of t, given earlier by Eq. (8), we had defined e as the difference in energy between the excited

[21] S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) **11**, 65 (1960).

[22] H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. **129**, 225 (1963).

intermediate state and the occupied initial state. That definition, therefore, holds good in Eq. (9) when $|s)$ happens to be an occupied state. If $|s)$ is an unoccupied state, one would think that in the definition of e, one should substitute $\epsilon(s)+\epsilon(m)$ in place of the initial occupied pair energy. This, however, is not true. The reason, popularly known as the effect of propagation "off-the-energy-shell," has been discussed at length by Bethe.[22] This once again gives rise to formal troubles akin to what was confronted in trying to define V in an arbitrary representation; namely, $(r|V|s)$ becomes dependent on other state labels besides $|r)$ and $|s)$. It will, however, be a good approximation at this stage to simulate the effect of off-energy-shell propagation for the case of unoccupied $|s)$ by adding an average energy-shift parameter δ to e. With this approximation $(r|V|s)$ does not become dependent on extraneous state labels, and hence the HF diagonalization equations can be written down meaningfully:

$$\sum_s (r|(T+V)|s)x_s = \epsilon x_r. \tag{10}$$

Once the matrix elements $(r|V|s)$ are well defined in terms of $(rm|t|sm)$ we can even convert the diagonalization equation (10) to harmonic-oscillator basis using the definition

$$(\alpha|V|\beta)=\sum_{r,s} x_\alpha{}^r (r|V|s) x_\beta{}^{s*}, \tag{11}$$

where the summations are over all states, occupied and unoccupied.

The reader is cautioned here to use the words "occupied" and "unoccupied" states exactly according to the conventions defined in Sec. I.

More practical details on the calculation of the t matrix are relegated to the Appendix II.

III. DETAILS OF THE HARTREE-FOCK CALCULATION

A. Choice of the Density Matrix

To obtain the solution of Eq. (4) we must first choose an initial density ρ. Once the density is chosen the HF matrix $\Gamma(\equiv T+V)$ can be diagonalized and the new density matrix obtained using Eq. (5b). The process is repeated until a self-consistent density is obtained. The choice of the initial density is very important for the following reason. It is clear that the definition (5a) of the HF potential V can be written in a short-hand notation as $V_1=\mathrm{Tr}_2 v_{12}\rho_2$ where the labels refer to the particles. The two-body potential v_{12} is a scalar under rotation, and is invariant under time-reversal and parity operations. It follows, therefore, that whatever symmetry property is incorporated into the density ρ with respect to the above three operations, gets reproduced in HF-potential V. The wave functions that are obtained from the resultant Γ will yield a density at the next iteration having the same symmetry property. Thus all the symmetry properties of the initial ρ are transmitted on to the final self-consistent solution. To get HF solutions with different types of symmetry properties one has, therefore, to start the iteration with various choices of ρ. The self-consistent ground-state energy in each such case represents a local minimum, and the lowest of all these minima correspond to the energetically most-favored ground-state wave function.

We first did a set of calculations with a completely arbitrary starting density without caring to build in any specific symmetry property. Nevertheless, we found that the self-consistent single-particle states in even-even ($N=Z$) nuclei occur in time-reversed pairs of good parity. The wave functions which are linear combinations of the states $|nljm)$, in general, contain all values of m between $-j$ and j.

Use of the Body-Fixed Axes

By a suitable rotation of the coordinate axes, the wave function can be transformed to a form where only terms with angular momentum projection quantum numbers "m" differing by two occur.

Bar-Touv and Kelson[18] have shown that this corresponds to working in the body-fixed axes, which implies imposing specific symmetry properties on the density matrix. To obtain the Hartree-Fock solution in the body-fixed frame we therefore demand the density matrix connect states with angular-momentum projection $m=\frac{1}{2}$ to states with $m=-\frac{3}{2}$ and $\frac{5}{2}$, while those with $m=-\frac{5}{2}$, $-\frac{1}{2}$, and $\frac{3}{2}$ are connected with each other. Corresponding to these two subspaces the density matrix can then be divided into ρ_1 and ρ_2, which are related as follows through the time-reversal invariance.

Time-Reversal Invariance

It has been already stated that the self-consistent solutions do occur in time-revised pairs for $(N=Z)$ even-even nuclei, even when one starts the calculation with a general density matrix. Thus, the convergence can be improved by starting out with a density matrix that is invariant under time reversal. Applying the time-reversal operator $\mathbf{T}$ to ρ, we obtain

$$\langle nljm|\mathbf{T}^\dagger\rho\mathbf{T}|n'l'j'm'\rangle = (-1)^{j-m+j'-m'}\langle nlj,-m|\rho|n'l'j',-m'\rangle. \tag{12}$$

Therefore, $\mathbf{T}^\dagger\rho\mathbf{T}\equiv\rho$ requires

$$(nljm|\rho_2|n'l'j'm') = (-1)^{j-m+j'-m'}(nlj,-m|\rho_1|n'l'j'-m'). \tag{13}$$

By choosing the initial density matrix ρ_1 in the subspace of $(m=-\frac{3}{2},\frac{1}{2},\frac{5}{2})$ and also demanding that the density ρ_2 is given by Eq. (13), we obtain self-consistent solutions in the body-fixed axes with the time-reversal invariance built in from the very outset. The only re-

striction that has to be satisfied in choosing ρ_1 is $\mathrm{Tr}\rho = 2\ \mathrm{Tr}\rho_1 = 2\times\mathrm{Tr}\ \rho_2 = A$, the number of nucleons. At subsequent stages of the iteration this is automatically satisfied.

Behavior under Rotation

The choice of a general ρ_1 which contains mixing of different m quantum numbers ($\Delta m = \pm 2$) corresponds to a very general intrinsic shape of the nucleus. All it presupposes is the presence of a quantization axis, the z axis shall we say, and a symmetry under rotation of 180° about the y axis. Applying further restrictions to the initial choice of the density matrix, we may generate solutions which are spherical and axially symmetric.

If the density has an axis of symmetry (which we may conveniently label as the z axis), then clearly it cannot have matrix elements connecting different m values; only the (nlj) quantum numbers mix. The matrix elements connecting different (nlj), however, depend on what m quantum number these states correspond to. On the other hand, a spherical density, being rationally invariant, cannot mix different l, j, and m quantum numbers; it mixes different n quantum numbers and the matrix elements have to be independent of m.

In our calculations the radial mixing is restricted to the $1s$ and $2s$ states. Thus, the asymptotic form of the Hartree-Fock field and the wave functions is Gaussian. If the expansion of the HF wave function is not truncated with respect to the sum over the principal quantum number n, the solutions would be independent of the oscillator constant b (cf. Baranger[17] and Kerman, Svenne, and Villars[14]): $b^2 = \hbar/M\omega$ and b makes r dimensionless in the oscillator wave function. Because of the limited basis used in the present calculation, the radial dependence of the HF field and the wave functions are characterized by the oscillator constant b. Therefore, b was chosen so that the rms radii agreed with the results from electron scattering. Since we are primarily interested in calculating the gain in the binding energy as the self-consistent field is allowed to deform, we do not consider the restricted radial dependence to be serious. Further remarks about the truncation of the expansion ψ_{HF} in terms of oscillator wave function is included in Sec. V.

Parity Mixing

We found, for an arbitrary initial density connecting states of opposite parity, that in all cases the ultimate self-consistent solutions were of good parity. We now show that our calculations include the possibility of generating mixed parity solutions.

Consider the definition (5a) of the HF potential V. It is clear that the states α and β are required to be of same (opposite) parity depending on whether γ and δ have the same (opposite) parity. This follows from the conservation of parity in the matrix elements of v. Thus, starting with a density that mixes parity, we should be able to reproduce self-consistent wave functions of mixed parity. Further insight is obtained by writing the multipole expansion for the potential v in the two-body matrix elements that enter into the calculation of V. For a central potential, we have

$$v(|r_1-r_2|)=\sum_{L,M} V_L(r_1,r_2)Y_M{}^{L*}(\hat{r}_1)Y_M{}^{L}(\hat{r}_2)\,, \quad (14)$$

and hence $(\alpha\gamma|v|\beta\delta)_a$ contains factors of the type $(\alpha|Y_M{}^{L*}(\hat{r}_1)|\beta)(\gamma|Y_M{}^{L}(\hat{r}_2)|\delta)$ in the direct term, and $(\alpha|Y_M{}^{L*}(\hat{r}_1)|\delta)(\gamma|Y_M{}^{L}(\hat{r}_2)|\beta)$ in the exchange term. It is clear, therefore, that the direct term mixes parity in the HF potential through the odd multipoles, and the exchange term through both odd and even multipoles.

The tensor potential may also be written in multipoles. Each $Y_M{}^L$ now appears multiplied by a $\boldsymbol{\sigma}\cdot\hat{r}$. Since the latter changes parity, the role of the odd and even multipoles will now be reversed.

Since, however, good-parity solutions were found to be energetically favored (at least for the two-body potential that we have been working with), we chose for our final calculations an initial ρ that conserves parity. This achieved faster convergence. Kerman, Bassichis, and Svenne[23] have made very detailed investigation of the role of parity mixing in HF calculations. In particular, they explore the effect of changing the strength of the tensor potential to achieve a lowering of the parity-mixed HF solution below the good-parity solution.

B. Nuclear Deformation

The self-consistent wave functions allow one to express the nuclear deformation quantitatively in terms of parameters, familiar to the nuclear collective model.

We first evaluate the quadrupole moments:

$$\langle Q_M\rangle=\left(\frac{16\pi}{5}\right)^{1/2}\langle\sum_{i=1}^{A} r_i{}^2Y_M{}^2(\theta_i\phi_i)\rangle \quad (15a)$$

using the HF determinantal wave function.

In the body-fixed axes, the $M=\pm 1$ terms are zero due to reflection symmetry. Only Q_0, Q_2, and Q_{-2} are nonvanishing with $Q_2=Q_{-2}$.

We characterized the nuclear shape by the elongation parameter β and the angle of asymmetry γ. Expanding the deformed nuclear surface to lowest order, as

$$R=R_0[1+\sum_M a_M Y_M{}^2(\theta,\phi)]\,,$$

the collective model gives, to first order in a_M,

$$\langle Q_M\rangle=\frac{3}{(5\pi)^{1/2}}ZR_0{}^2a_M\,. \quad (15b)$$

Using the calculated values of Q_M, Eq. (15b) and the

[23] A. K. Kerman, W. H. Bassichis, and J. P. Svenne, Bull. Am. Phys. Soc. **11**, 304 (1966).

relations,

$$a_0=\beta\cos\gamma, \quad \text{and} \quad a_2=a_{-2}=\frac{1}{\sqrt{2}}\beta\sin\gamma, \qquad (15c)$$

we evaluated the deformation β and the angle of asymmetry γ. It should be mentioned here that only values of γ in the range 0°–60° are important. Higher values of γ mean a repetition of the same ellipsoidal shape, with the labeling of the x, y, z axes interchanged.[24]

C. Method of Lagrange Multipliers

The calculations were first carried out starting with an initial density which had unity for the elements of ρ_1 and ±1, for the elements of ρ_2 (ρ_2 being the time reversed of ρ_1). For all nuclei the program converged to give a self-consistent field. In order to confirm that the calculation had converged to the lowest minimum we were forced to use a method that permits the determination of the energy as a function of β and γ. The method of Lagrange multipliers, used extensively by Bassichis and Kerman,[16] has been used for this purpose.

The Hartree-Fock approximation requires $\delta\langle\psi|H|\psi\rangle$ to be zero with the constraint that $\langle\psi|\psi\rangle$ be normalized. This leads to the variational equation

$$\delta[\langle\psi|H|\psi\rangle-\epsilon\langle\psi|\psi\rangle]=0, \qquad (16)$$

where ϵ is a Lagrange multiplier to take into account the single constraint mentioned above. It has been already shown in Sec. II that using a determinantal form for ψ, and single-particle wave functions in the form (2a), yields the HF equation (4). The constant ϵ, which is the energy eigenvalue, is the simplest Lagrange multiplier.

In the present case we want to evaluate the energy as a function of β and γ. We therefore seek a deformed ψ in the minimization of $\langle\psi|H|\psi\rangle$ subject to further constraints:

$$(\psi|Q_M|\psi)=q_M, \quad M=0 \text{ and } \pm2, \qquad (17)$$

where Q_M is the quadrupole operator in the body-fixed frame, and q_m is its specified value.

We are thus required to solve

$$\delta[(\psi|H|\psi)-\epsilon(\psi|\psi)-\lambda_0(\psi|Q_0|\psi) -\lambda_2(\psi|Q_2+Q_{-2}|\psi)]=0, \qquad (18)$$

where λ_M are the new Lagrange multipliers multiplying the additional constraints. Substituting the expression for the wave function in terms of harmonic-oscillator wave functions, Eq. (2a), and carrying out the variation we are led to the following modified HF equation:

$$\sum_\beta [T+V-\lambda_0Q_0-\lambda_2(Q_2+Q_{-2})]_{\alpha\beta}x_\beta{}^i=\epsilon_i x_\alpha{}^i. \qquad (19)$$

The terms Q_M in Eq. (19) are the driving terms for nuclear deformation; the amount of deformation they can force is dependent on the numerical value used for the Lagrange multipliers λ_M. Our previous observation that the symmetry properties of the initial density is propagated unaltered through the iterations is no longer true for Eq. (19). Even if we calculate V with a starting spherical density (and hence V spherical), the presence of the terms Q_M in Eq. (19) yields nonspherical solution for the wave functions $x_\alpha{}^i$, and hence the density, and V calculated for the next iteration becomes nonspherical. For Q_0 finite and $Q_2=Q_{-2}=0$, V is axially symmetric.

We expressed λ_0 and λ_2 as functions of λ and θ:

$$\lambda_0=\lambda\cos\theta \quad \text{and} \quad \lambda_2=(\lambda/\sqrt{2})\sin\theta,$$

and generated the HF field for $\lambda=-22$ to 22 and $\theta=0°$ to 60°. For each value of λ and θ the corresponding ψ enables one to calculate q_M (which alone have physical significance as the quadrupole moments of the nucleus), and the deformation β and angle of asymmetry γ by Eqs. (15b) and (15c).

Although it is possible to increase or decrease the driving terms continuously through the Lagrange multipliers λ_M, the response of the system, which is measured by the corresponding changes in q_M, is found to be rather sluggish.

Since the expectation values of Q_M are not linearly related to λ_M, one obtains solutions for restricted values of q_M. As the parameters λ and θ vary, the expectation values q_M of Q_M are given in a few isolated domains. Table I, which gives the results for ^{24}Mg, demonstrates this fact. Each isolated domain corresponds to one local minimum of the ground-state energy. The results show that the Lagrange multiplier method cannot be used to determine the energy surface as a continuous function of β and γ. However, they can be used to drive the system from one local minimum to another on the energy surface. We found that once the system has been driven into a local minimum with the help of Lagrange multipliers, then the corresponding density can be very conveniently used to start the iterative solution of the original HF equation (4) [in other words, Eq. (19) with $\lambda_M=0$]; this procedure very quickly leads us to the neighboring minimum point on the ground-state energy versus the deformation curve.

It was further noticed that the driving of the ground-state energy from one minimum to another is intimately related with the crossing of single-particle levels near the Fermi surface. This suggests a possible alternative way of exploring all the minima of the energy. Instead of constructing a ground-state wave function, at each iteration, by filling up the lowest A levels (A = number of nucleons), one can always choose to have the particles in a given set of levels, and iterate the original HF equation (4) to obtain the corresponding self-consistent solution and the ground-state energy. Then one should exhaust all possible ways of allotting particles to

[24] A. Bohr and B. R. Mottelson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **27**, 1 (1953).

TABLE I. Hartree-Fock solutions for ^{24}Mg as a function of λ and θ^0. BE/A is the binding energy per particle in MeV and $\langle r^2Y_0^2\rangle$ and $\langle r^2(Y_2^2+Y_{-2}^2)\rangle$ are in F^2.

θ° / λ	0° $\langle r^2Y_0^2\rangle$	0° $\langle r^2(Y_2^2+Y_{-2}^2)\rangle$	0° BE/A	20° $\langle r^2Y_0^2\rangle$	20° $\langle r^2(Y_2^2+Y_{-2}^2)\rangle$	20° BE/A	40° $\langle r^2Y_0^2\rangle$	40° $\langle r^2(Y_2^2+Y_{-2}^2)\rangle$	40° BE/A
−22.0	−26.207	0	−5.292	−26.197	−0.029	−5.296	−16.387	−12.045	−4.346
−18.0	−26.196	0	−5.310	−26.186	−0.028	−5.314	−16.396	−12.013	−4.379
−14.0	−26.178	0	−5.334	−26.167	−0.027	−5.339	−16.409	−11.971	−4.416
−10.0	−26.145	0	−5.366	−26.132	−0.026	−5.371	−16.418	−11.914	−4.460
−6.0	−26.074	0	−5.411	−26.059	−0.024	−5.416			
−4.0	−26.001	0	−5.442	−13.291	−7.747	−6.818	−13.129	−8.076	−6.778
				−13.016	−7.753	−6.879	−13.034	−8.023	−6.828
−2.0	−14.250	0	−6.462	−12.755	−7.731	−6.909	−12.835	−7.936	−6.883
−1.0	−13.411	0	−6.566	−12.529	−7.704	−6.923	−12.628	−7.850	−6.911
−0.5	−12.899	0	−6.598	0	0	−6.205	−12.447	−7.781	−6.924
0	0	0	−6.205	15.753	3.733	−6.924	0	0	−6.205
				15.932	3.808	−6.911	15.699	3.822	−6.923
0.5	15.734	0	−6.758	16.135	3.895	−6.883	15.845	3.947	−6.909
1.0	15.947	0	−6.745	16.341	3.975	−6.828	16.001	4.097	−6.878
2.0	16.188	0	−6.716	16.453	4.006	−6.778	16.129	4.270	−6.817
4.0	16.426	0	−6.659						
				22.798	4.102	−4.461	13.058	15.946	−5.416
6.0	22.901	0	−4.069	22.862	4.069	−4.417	13.097	15.990	−5.371
10.0	22.983	0	−4.016	22.907	4.040	−4.380	13.116	16.011	−5.338
14.0	23.055	0	−3.935	22.940	4.015	4.348	13.127	16.022	−5.314
18.0	23.074	0	−3.904				13.134	16.022	−5.296
22.0	23.074	0	−3.904						
0	−12.182	0	−6.612	−12.096	−7.631	−6.931*			
0	−25.458	0	−5.502						
0	15.328	0	−6.765	15.394	3.592	−6.931*			

alternative levels near the Fermi surface, and get the self-consistent solution for each such choice. The lowest of these solutions is the true HF ground-state solution. The other solutions represent excited intrinsic states. This method, however, yields only a few isolated points on the energy surface (versus the deformation), while the Lagrange multiplier method generates parts of the energy surface in the neighborhood of the above points. Moreover, the Lagrange multiplier method automatically causes the shift from one set of occupied levels to another without requiring any intuition in making the choice.

It may appear that the single-particle spectrum, obtained by solving Eq. (19), should need corrections corresponding to the extra quadrupole terms before they can be used in setting up the HF determinant. The manner of derivation of this equation will, however, tell us not to do this. It was proved that the determinantal ground-state wave function, built with the help of the single-particle spectrum and wave functions obtained from Eq. (19), does really minimize, subject to certain given values of the quadrupole moments, the ground-state energy $\langle\psi|H|\psi\rangle$, where H is the *original* Hamiltonian.

IV. NUMERICAL RESULTS

The calculations were carried out for the $4n$ nuclei, $8\leq A\leq 40$. The HF fields were generated for λ in the range -22 to 22 and θ between 0° and 60°. In general, for larger values of λ, either the calculations failed to converge, or the $1s$ state was found to be bound very strongly (>120 MeV). Such solutions were considered unphysical. For θ in the range 0° to 60° all possible axially asymmetric shapes are possible; $\theta>60°$ corresponds to a rotation of the body fixed axes. In the calculations the initial density matrix was taken to be spherical plus the admixtures due to the driving terms λ_0Q_0 and $\lambda_2(Q_2+Q_{-2})$. Hence λ was increased from 0 to 22 and decreased from 0 to -22. To illustrate the procedure we followed we present the results for ^{24}Mg first. In Table I we give the values of $r^2Y_0^2$, $r^2[Y_2^2+Y_{-2}^2]$ (i.e., β and γ), and the binding energy per particle (BE/A), as a function of λ and θ. For $\theta=0$, four axially symmetric solutions were found. The minima corresponding to $\langle r^2Y_0^2\rangle\approx-12$ F^2 (oblate) and $+15$ F^2 (prolate) correspond to the configurations $(1d_{5/2}{}^{\pm5/2})^2\times(1d_{3/2}{}^{\pm3/2})^{-2}$ and $(1d_{5/2}{}^{\pm5/2})^{-2}(1d_{5/2}{}^{\pm3/2})^2$, respectively. The solution with $\langle r^2Y_0^2\rangle\approx-26$ F^2 has the $1d_{5/2}{}^{\pm5/2}$ states filled, while the $1d_{5/2}{}^{\pm3/2}$ shell is populated at the expense of the $1p_{3/2}{}^{\pm1/2}$ and $1p_{1/2}{}^{\pm1/2}$ states. The discontinuities in the expectation values of $r^2Y_0^2$ and $r^2(Y_2^2+Y_{-2}^2)$ occur when the single-particle levels cross and the particles occupy different states.

In all cases, we found, when driving the system from one minimum to another, the system possessed an intrinsic inertia against changing its shape. Consider, for example, prolate deformations. The expectation value for $r^2Y_0^2=15.734$ F^2 and that of $r^2(Y_2^2+Y_{-2}^2)=0$. Adding a small amount of the axially asymmetric driving term, $\theta=5°$, we found the value of $r^2(Y_2^2+Y_{-2}^2)=3.568$ F^2. For $\theta=20°$ and 40°, the value of $r^2(Y_2^2+Y_{-2}^2)$

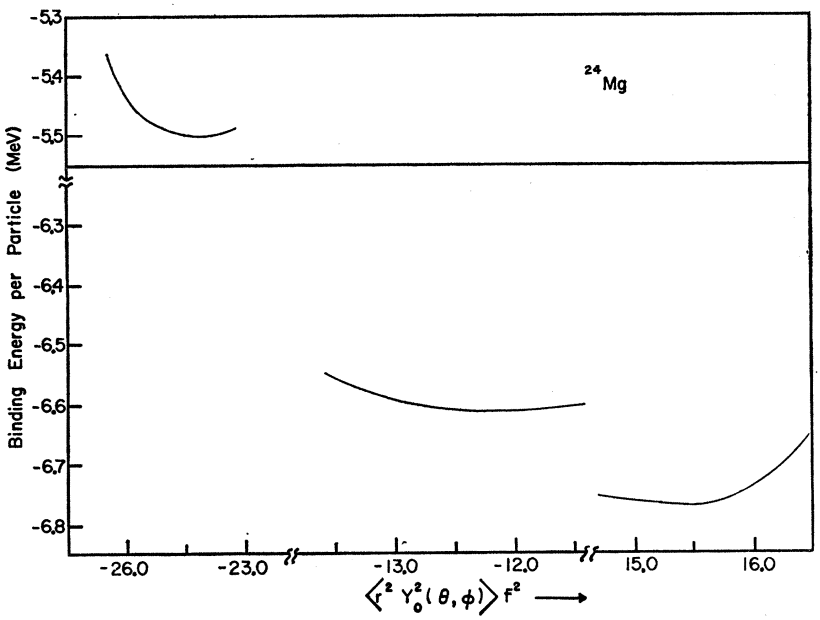

FIG. 1. Variation of the binding energy per particle as a function of $\langle r^2 Y_0^2(\theta\phi)\rangle$ for axially symmetric deformations in ^{24}Mg. Note that the coordinate axis is broken.

$=3.733$ and 3.822 F^2, respectively, while the value for the absolute minimum is 3.592 F^2. The system is, therefore, very stable near the minimum. With only a small admixture of an axially asymmetric term to the density matrix, the calculation iterates to nearly the absolute minimum. We also point out that the system is always driven past the local minima by λ_0 and λ_2 (i.e., for $\lambda=0.5$, 1.0, 2.0, and 4.0 the BE/A decreases). Therefore, once the local minimum ($r^2Y_0^2=15.328$ F^2) was obtained we used the resulting density as the starting density for further calculation and drove the system in the opposite direction (i.e., $\lambda=-0.5$, -1.0, -1.5, -2.0). We then obtained the HF solution for $\beta \gtrless \beta_{\min}$, i.e., $\langle r^2Y_0^2\rangle \gtrless \langle r^2Y_0^2\rangle_{\min}$. We give the results in Fig. 1. The last three lines of Table I give the various absolute local minima. The solutions denoted by an asterisk are related by a rotation of the frame of reference. In Table II, we give the single-particle spectrum for the spherical, oblate, prolate, and absolute minima. There is no $1p_{3/2}$, $1p_{1/2}$ state splitting when ^{24}Mg is constrained to be spherical; however, the absolute minimum does give a reasonable splitting of the p levels. The wave functions for the absolute minimum and for the prolate minimum are given in Table III.

The only other nucleus, besides ^{24}Mg, which was found to be axially asymmetric was ^{32}S. In Table IV, we summarize the minima occurring in ^{32}S and give the wave functions for the absolute minimum. It is reassuring that the HF approximation gives axially asymmetric shapes for ^{24}Mg and ^{32}S which are the 8-particle and 8-hole nuclei, respectively, in the s-d shell. The remaining nuclei were found to be axially symmetric, except for ^{16}O and ^{40}Ca, which are spherical.

The most interesting axially symmetric nucleus is ^{28}Si, where we found three minima corresponding to oblate, prolate, and approximately spherical HF fields. We expect the prolate and oblate fields since ^{28}Si is midway between the closed shells of ^{16}O and ^{40}Ca. Also, if the j-j coupling is valid, ^{28}Si would correspond to the $^1d_{5/2}$ subshell being occupied, and we would then expect to find a minimum corresponding to a spherical field. The results are illustrated in Fig. 2 and the wave functions are given in Table V.

The case of ^{20}Ne is also of considerable interest. We find that the absolute minimum is axially symmetric (prolate); however, a minimum corresponding to an asymmetric field was found. The minima occurring in ^{20}Ne are given in Table VI as are the wave functions.

In Table VII the HF single-particle energies for ^{16}O and ^{40}Ca are given along with the experimental values. The $1p_{3/2}$, $1p_{1/2}$ splitting in ^{16}O is in good agreement

TABLE II. Single-particle energy levels in ^{24}Mg in MeV.

Level \ BE/A	Spherical −6.205	Oblate −6.612	Prolate −6.765	Asymmetrical −6.931
		Occupied levels		
$1s_{1/2}{}^{\pm 1/2}$	−62.978	−61.267	−65.042	−64.650
$1p_{3/2}{}^{\pm 3/2}$	−33.849	−37.779	−30.303	−32.066
$1p_{3/2}{}^{\pm 1/2}$	−33.849	−36.267	−39.857	−39.115
$1p_{1/2}{}^{\pm 1/2}$	−33.845	−25.547	−28.445	−26.385
$1d_{5/2}{}^{\pm 5/2}$	−9.128	−14.875	−5.118	−6.310
$1d_{5/2}{}^{\pm 3/2}$	−9.128	−11.489	−10.486	−13.471
		Unoccupied levels		
$1d_{5/2}{}^{\pm 1/2}$	−9.128	−9.142	−16.191	−16.556
$2s_{1/2}{}^{\pm 1/2}$	−4.862	−5.053	−2.323	−2.155
$1d_{3/2}{}^{\pm 3/2}$	−6.815	−3.877	−0.512	−0.546
$1d_{3/2}{}^{\pm 1/2}$	−6.815	−0.031	−8.941	5.124

TABLE III. Results for ^{24}Mg.

Energy (MeV)	$1s_{1/2}^{1/2}$	$1p_{3/2}^{-3/2}$	$1p_{3/2}^{1/2}$	$1p_{1/2}^{1/2}$	$1d_{5/2}^{-3/2}$	$1d_{5/2}^{1/2}$	$1d_{5/2}^{5/2}$	$2s_{1/2}^{1/2}$	$1d_{3/2}^{-3/2}$	$1d_{3/2}^{1/2}$
HF wave functions (absolute minimum); $\beta=0.324$, $\gamma=17°52'$, and $BE/A=-6.931$ MeV.										
Occupied levels										
−64.650	−0.9906				−0.0114	−0.0570	−0.0225	−0.1068	0.0204	0.0550
−39.115		0.0451	−0.8960	0.4418						
−32.066		−0.8900	0.1649	0.4252						
−26.385		0.4538	0.4123	0.7900						
−16.556	0.0078				0.2072	−0.8174	−0.0653	0.4798	0.1325	0.1918
−13.471	0.0012				−0.7705	0.0583	−0.0513	0.2777	−0.2231	0.5228
Unoccupied levels										
−6.310	0.0334				−0.3218	−0.4122	0.7388	−0.3450	−0.1108	−0.2198
−5.124	−0.0233				0.4075	0.3078	0.6165	0.1847	0.0818	0.5637
−2.155	0.1121				0.2074	−0.2443	−0.2522	−0.6663	−0.3139	0.5278
0.546	0.0667				−0.2249	−0.0277	−0.0555	−0.2902	0.9026	0.2053
HF wave functions; (prolate) $\beta=0.323$, $\gamma=0$, and $BE/A=-6.765$ MeV.										
Occupied levels										
−65.042	−0.9905					−0.0656		−0.1065		0.0575
−39.857			−0.8772	0.4802						
−30.303		1.0								
−28.445			0.4802	0.8772						
−16.191	0.0168					−0.7902		0.5118		0.3366
−10.486					0.9543				0.2990	
Unoccupied levels										
−8.941	−0.0228					0.5340		0.3075		0.7873
−5.118							1.0			
−2.323	0.1348					−0.2934		−0.7951		0.5134
−0.512					0.2990				−0.9543	

with the results of quasi-(p,p') scattering.[25] However, for ^{16}O the HF approximation overbinds the p states by approximately 4 MeV, while in ^{40}Ca the calculations overbind the d levels by 5 MeV and the s level by ≈ 9 MeV. In Table VIII we give the single-particle energies for the remaining $4n$ nuclei when the fields are constrained to be spherical. We see from Table VIII that when ^{24}Mg is constrained to be spherical there is no $1p_{3/2}$, $1p_{1/2}$ splitting. However, from Table III we see that for the asymmetric field the p state splitting is reasonable. When ^{28}Si and ^{32}S are restricted to having spherical fields the $1p_{1/2}$ state lies below the $1p_{3/2}$ state.

It is clear that deformed HF fields must be allowed, to account for the level splitting and binding energy,

TABLE IV. Results for ^{32}S.

Energy (MeV)	Shape	$r^2Y_2^0$ (F^2)	$r^2(Y_2^2+Y_2^{-2})$ (F^2)	BE/A (MeV)	Energy gap (MeV)
Hartree-Fock minima.					
	Spherical	0	0	−7.602	0.570
	Oblate	−6.933	0	−8.004	3.673
	Asymmetrical	*−14.061*	*−4.437*	*−8.129*	*6.063*
	Prolate	12.022	0	−8.026	3.043

HF wave functions, $\beta=-0.190$, $\gamma=23°33'$, and $BE/A=-8.128$ MeV.

	$1s_{1/2}^{1/2}$	$1p_{3/2}^{-3/2}$	$1p_{3/2}^{1/2}$	$1p_{1/2}^{1/2}$	$1d_{5/2}^{-3/2}$	$1d_{5/2}^{1/2}$	$1d_{5/2}^{5/2}$	$2s_{1/2}^{1/2}$	$1d_{3/2}^{-3/2}$	$1d_{3/2}^{1/2}$
−74.489	−0.9957				0.0063	0.0431	0.0153	−0.0678	−0.0206	−0.0381
−48.303		0.8465	0.3679	0.3877						
−44.342		−0.5275	0.6732	0.5182						
−37.799		0.0719	0.6432	−0.7623						
−23.481	0.0034				0.0784	0.1532	0.9409	0.2895	−0.0158	−0.0320
−21.517	−0.0015				−0.7242	−0.4933	0.2347	−0.3070	0.2537	−0.1363
−18.753	−0.0101				−0.4519	0.5654	−0.1968	0.4547	0.3953	−0.2725
−16.336	−0.0070				−0.2043	−0.2338	−0.0945	0.3955	−0.7221	−0.4656
−10.273	−0.0465				0.4133	−0.5368	−0.0734	0.4014	0.5063	−0.3406
−6.683	0.0792				0.2293	0.2622	0.0793	−0.5415	0.0301	−0.7563

[25] H. Tyren, S. Kullander, O. Sundberg, R. Ramachandran, P. Isacsson, and T. Berggren, Nucl. Phys. **79**, 321 (1966).

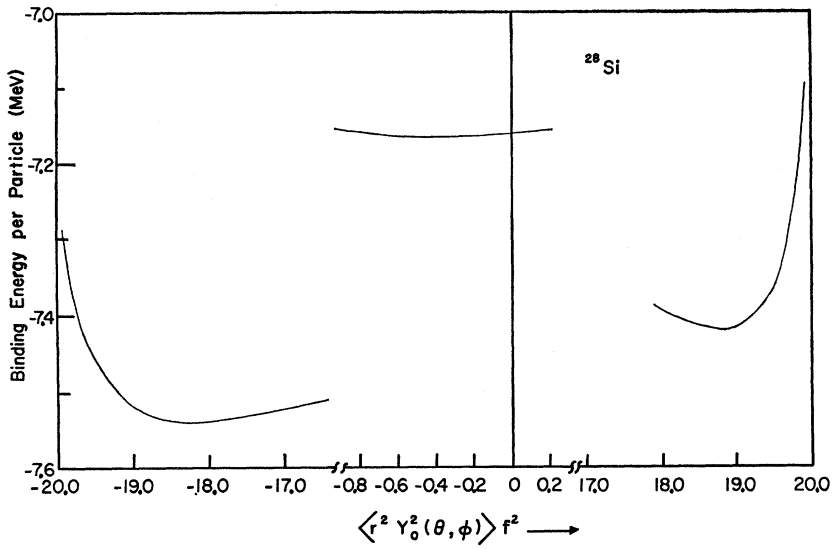

FIG. 2. Variation of the binding energy per particle as a function of $\langle r^2 Y_0^2(\theta\phi)\rangle$ for axially symmetric deformation in ^{28}Si. Note that the coordinate axis is broken.

TABLE V. Results for ^{28}Si.

Energy (MeV)	$1s_{1/2}{}^{1/2}$	$1p_{3/2}{}^{-3/2}$	$1p_{3/2}{}^{1/2}$	$1p_{1/2}{}^{1/2}$	$1d_{5/2}{}^{-3/2}$	$1d_{5/2}{}^{1/2}$	$1d_{5/2}{}^{5/2}$	$2s_{1/2}{}^{1/2}$	$1d_{3/2}{}^{-3/2}$	$1d_{3/2}{}^{1/2}$
HF wave functions; $\beta=-0.282$, $\gamma=0$, and $BE/A=-7.539$ MeV. Occupied levels										
−70.617	0.9910					−0.0676		0.1004		0.0568
−42.978		1.0								
−40.826			0.6991	0.7151						
−29.633			0.7151	−0.6991						
−19.862							1.0			
−17.476	−0.0157					0.6143		0.7330		−0.2916
−16.268					−0.6823				0.7310	
Unoccupied levels										
−7.379					0.7310				0.6823	
−6.760	0.0626					0.7430		−0.4135		0.5225
−1.813	0.1170					0.2568		−0.5307		−0.7992
HF wave function; $\beta\approx-0.002$, $\gamma=0$, and $BE/A=-7.163$ MeV. Occupied levels										
−66.646	0.9995					0.0015		0.0292		0.0101
−39.942			0.5930	0.8052						
−39.421		1.0000								
−39.041			0.8052	−0.5930						
−16.774					0.9716				0.2365	
−16.140	0.0071					−0.7810		0.0108		−0.6244
−13.235							1.0000			
Unoccupied levels										
−11.458					0.2365				−0.9716	
−7.947	0.0054					0.6240		0.0524		−0.7796
−7.449	0.0296					0.0243		0.9981		−0.0474
HF wave function; $\beta=0.284$, $\gamma=0$, and $BE/A=-7.418$ MeV. Occupied levels										
−69.556	−0.9923					−0.0588		−0.0855		0.0688
−45.436			−0.8853	0.4651						
−36.153		1.0000								
−31.795			0.4651	0.8853						
−20.984	0.0117					−0.8447		0.5256		0.1004
−18.749					0.9399				0.3416	
−13.324	0.0019					0.3549		0.4098		0.5403
Unoccupied level										
−9.350							1.000			
−4.502	0.1239					−0.3963		−0.7406		0.5283
−2.665					0.3416				−0.9399	

TABLE VI. Results for ^{20}Ne.

Energy (MeV)	Shape	$\langle r^2Y_2^0\rangle$ (F^2)	$\langle r^2(Y_2^2+Y_2^{-2})\rangle$ (F^2)	BE/A (MeV)	Energy gap (MeV)
		Hartree-Fock minima.			
	Spherical	0.000	0.0	−6.026	
	Oblate	−6.652	0.0	−6.168	0.095
	Oblate	−20.560	0.0	−4.781	4.146
	Prolate	12.336	0.0	−6.601	7.423
	Asymmetric	19.078	8.016	−4.908	3.401
	Asymmetric	3.232	3.958	−6.390	5.006

HF wave functions, (Prolate) $\beta=0.335$, $\gamma=0$, and $BE/A=-6.601$ MeV.

	$1s_{1/2}{}^{1/2}$	$1p_{3/2}{}^{-3/2}$	$1p_{3/2}{}^{1/2}$	$1p_{1/2}{}^{1/2}$	$1d_{5/2}{}^{-3/2}$	$1d_{5/2}{}^{1/2}$	$1d_{5/2}{}^{5/2}$	$2s_{1/2}{}^{1/2}$	$1d_{3/2}{}^{-3/2}$	$1d_{3/2}{}^{1/2}$
					Occupied levels					
−59.171	−0.9894					−0.0455		−0.1315		0.0425
−32.216			−0.9202	0.3915						
−26.315		1.0000								
−22.018			0.3915	0.9202						
−12.263	−0.0073					−0.7976		0.4574		0.3931
					Unoccupied levels					
−4.839					−0.9856				−0.1690	
−2.557							1.0000			
−1.488	−0.1030					0.5930		0.6962		0.3912
1.294	0.1025					0.1005		−0.5374		0.8310
3.810					−0.1690				0.9856	

for nuclei between closed shells. For ^{24}Mg the gain in BE/A when the field is allowed to change from spherical to axially asymmetric is 0.726 MeV, while the gain, when the field is allowed to change from axially symmetric to asymmetric is 0.166 MeV.

In Tables IX and X, we give the wave functions for ^{8}Be and ^{12}C, respectively, while in Table XI, we present a summary of the results for the $4n$ nuclei. Figure 3 illustrates the variation of β with mass number. The agreement with the predictions of the collective model is satisfactory. Figure 4 gives the binding energy of the $1s_{1/2}{}^{\pm1/2}$, $1d_{5/2}{}^{\pm5/2}$, and $1d_{5/2}{}^{\pm1/2}$ levels as a function of A.

TABLE VII. Self-consistent single-particle energies in ^{16}O and ^{40}Ca, in MeV.

	^{16}O	^{40}Ca	^{16}O data	^{40}Ca data
$1s_{1/2}$	−52.783	−62.408		
$1p_{3/2}$	−23.309	−39.579	−19.0	
$1p_{1/2}$	−17.568	−36.952	−12.4	
$1d_{5/2}$	−0.993	−21.111		−15.5
$1d_{3/2}$	6.004	−17.159		−8.3
$2s_{1/2}$	1.499	−16.358		−11.6
BE/A	−6.775	−7.506		

TABLE VIII. Single-particle binding energies for spherical fields in MeV.

(State)	^{8}Be	^{12}C	^{20}Ne	^{24}Mg	^{28}Si	^{32}S
$1s_{1/2}$	−44.040	−60.680	−57.806	−62.978	−68.295	−78.534
$1p_{3/2}$	−5.650	−16.321	−28.587	−33.849	−39.102	−43.308
$1p_{1/2}$	−1.509	−16.517	−25.720	−33.844	−41.946	−44.382
$1d_{5/2}$	16.138	9.558	−5.067	−9.128	−13.177	−16.482
$1d_{3/2}$	21.688	14.313	−0.414	−6.818	−13.207	−15.912
$2s_{1/2}$	13.021	8.233	−1.734	−4.862	−7.909	−16.502
BE/A	−2.780	−5.548	−6.026	−6.205	−6.916	−7.602

It is seen that the binding of the $1s_{1/2}{}^{\pm1/2}$ levels increases with A in agreement with the results from $(e,e'p)$ experiments.[26]

V. DISCUSSION—CONCLUSION

We have shown that the HF approximation, for the $4n$ nuclei, $A<40$, gives results, in reasonable agreement with experiment, provided the field is permitted to be deformed (axially symmetric or asymmetric). The results of the numerical calculation using the singular Yale potential are encouraging. However, we would like to point out several features of the calculation which are open to question.

Firstly, in the expansion of the HF wave functions ψ_{HF} in terms of oscillator wave functions, only the $1s$, $2s$, $1p$, and $1d$ functions have been included. It has been shown,[14] for the closed-shell nuclei O^{16} and Ca^{40} with nonsingular potentials, that harmonic-oscillator wave functions containing at least 3 nodes should be included in the HF calculation of the binding energy; with further increases in the number of nodes the binding energy and rms radius of the nucleus gradually tend to be independent of the oscillator well parameter b. It may appear, since we do not include the oscillator functions with higher number of nodes that our results are in error. We would like to point out that the situation is a bit ambiguous when singular potentials are used which require higher-order terms to be included in evaluating the effective interaction. It has been pointed out in the introduction that in calculating the latter the effect of exciting a pair of nucleons to very high-

[26] U. Amaldi, Jr., G. Campos Venuti, G. Cortellessa, C. Fronterotta, A. Reale, P. Salvadori, and P. Hillman, Phys. Rev. Letters 13, 341 (1964).

TABLE IX. ^{8}Be HF wave functions; $\beta=0.786$, $\gamma=0$, and $BE/A=-5.506$ MeV.

Energy (MeV)	$1s_{1/2}{}^{1/2}$	$1p_{3/2}{}^{-3/2}$	$1p_{3/2}{}^{1/2}$	$1p_{1/2}{}^{1/2}$	$1d_{5/2}{}^{-3/2}$	$1d_{5/2}{}^{1/2}$	$1d_{5/2}{}^{5/2}$	$2s_{1/2}{}^{1/2}$	$1d_{3/2}{}^{-3/2}$	$1d_{3/2}{}^{1/2}$
					Occupied levels					
−40.744	−0.9764					−0.1452		−0.0714		0.1429
−18.566			−0.8701	0.4930						
					Unoccupied levels					
−0.130		1.000								
6.865			0.4930	0.8701						
8.608	0.0877					−0.8043		0.5830		0.0737
12.050					0.9337				0.3580	
17.287	−0.1523					0.5641		0.8091		−0.0628
20.149							1.0000			
21.523	0.1254					0.1172		0.0184		0.9850
26.353					0.3580				−0.9337	

TABLE X. ^{12}C HF wave functions; $\beta=-0.343$, $\gamma=0$, and $BE/A=-7.039$ MeV.

Energy (MeV)	$1s_{1/2}{}^{1/2}$	$1p_{3/2}{}^{-3/2}$	$1p_{3/2}{}^{1/2}$	$1p_{1/2}{}^{1/2}$	$1d_{5/2}{}^{-3/2}$	$1d_{5/2}{}^{1/2}$	$1d_{5/2}{}^{5/2}$	$2s_{1/2}{}^{1/2}$	$1d_{3/2}{}^{-3/2}$	$1d_{3/2}{}^{1/2}$
					Occupied levels					
−55.522	0.9882					−0.0977		0.0714		0.0939
−24.238		1.0000								
−21.230			0.7187	0.6953						
					Unoccupied levels					
−2.381			0.6953	−0.7187						
2.078							1.0000			
6.368					−0.9009				0.4339	
7.216	−0.0016					0.6333		0.7685		0.0916
14.012	0.0819					0.7028		−0.6195		0.3399
16.222					0.4339				0.9009	
19.932	0.1294					0.3090		−0.1434		−0.9313

TABLE XI. Results of Hartree-Fock calculation for the $4n$ nuclei, $A\leq 40$.

	^{8}Be	^{12}C	^{16}O	^{20}Ne	^{24}Mg	^{28}Si	^{32}S	^{40}Ca
Binding energy per particle (MeV)	−5.507	−7.039	−6.775	−6.601	−6.931	−7.539	−8.128	−5.706
Oscillator parameter b^2 (F^2)	2.3716	2.3716	3.100	3.100	3.100	3.100	3.100	4.36
Rms radius (F)	2.156	2.245	2.596	2.754	2.854	2.925	2.977	
β	0.786	−0.343	0	0.335	0.324	−0.282	−0.190	0
γ	0	0	0	0	17°52′	0	23°33′	0
Energy gap (MeV)	18.436	18.849	16.574	7.423	7.161	8.889	6.063	

lying intermediate states is considered to all orders. Such an effective potential should be diagonalized in a subset of states that lie near the Fermi surface. In particular, there should be no overlap between this subset of states and the excited intermediate states considered in the calculation of the effective interaction, because if there is an overlap, then the contributions of such intermediate states are doubly counted. Since the harmonic-oscillator states with 3–4 nodes are very high lying in energy, it would appear that they should be omitted from the subset chosen for diagonalization in order to avoid double counting.

We are, therefore, faced with two alternatives in the case of a singular potential. If the oscillator wave functions with higher number of nodes are included in the expansion of Hartree-Fock wave functions, then we can make the HF results independent of the oscillator parameter b, and we may claim that the spherically symmetric HF potential has also been self-consistently determined giving the correct asymptotic behavior (provided the number of nodes included is large enough) of the self-consistent wave functions. If, on the other hand, we wish to avoid the possibility of double counting the contribution of some intermediate states then the oscillator wave functions with large number of nodes should be expressly omitted in the expansion of HF wave functions. This, however, prevents the possibility of determining the spherical HF field too well, and yields radial functions with incorrect asymptotic behavior.

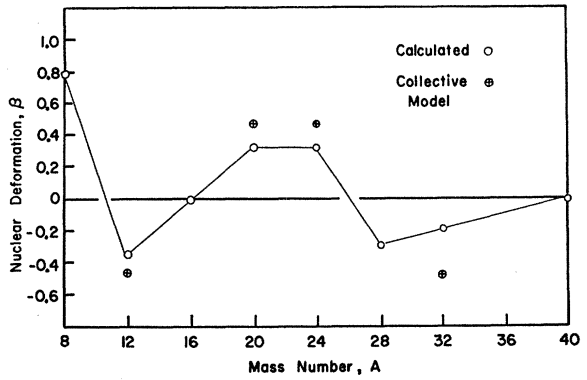

FIG. 3. Variation of the nuclear deformation β as a function of mass number.

Since we have mostly concerned ourselves with deformed nuclei, we did not lay the primary emphasis on being able to determine the spherical part of the HF field too accurately. The limited set of states we have used will be good enough for the self-consistent determination of the deformation. We have, therefore, decided in favor of the second alternative mentioned above.

The limited asymptotic radial dependence of our HF fields may cause up to 20% error in the moments $r^2Y_0^2$ and $r^2[Y_2^2+Y_{-2}^2]$. In our calculation this error could not be avoided. The values of β deduced from the HF field are less than the predictions of the collective model, as expected.

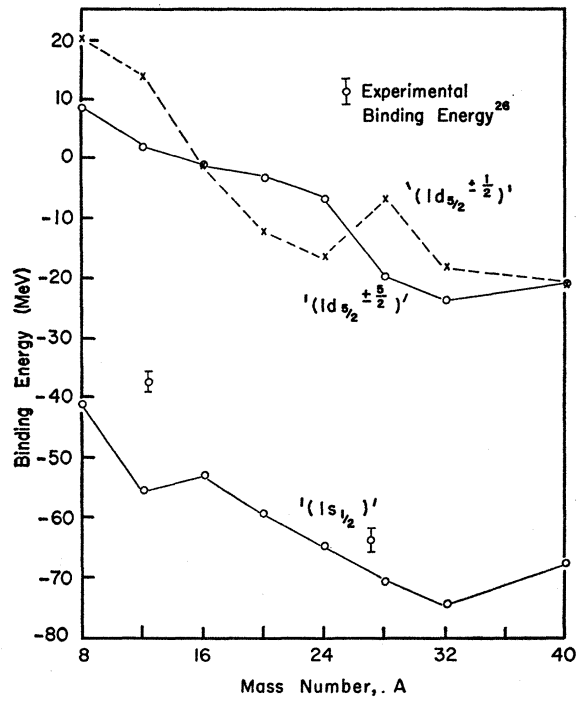

FIG. 4. Variation of the energy, for levels having the greatest $1s_{1/2}{}^{\pm 1/2}$, $1d_{5/2}{}^{\pm 5/2}$, and $1d_{5/2}{}^{\pm 1/2}$ amplitudes, as a function of mass number.

Another limitation of the present work is the neglect of Coulomb forces for the protons, and consequent treatment of neutrons and protons on an equal footing in $N=Z$ nuclei. We have also ignored the correction to the binding energy due to the center-of-mass motion. Both the Coulomb and center-of-mass effects have been calculated for O^{16} and Ca^{40} in Ref. 14 and found to make nearly equal and opposite contributions to the binding energy. Since our omission of wave functions with higher nodes has already made the calculated binding energies liable to some error, we did not think it worthwhile to calculate such small corrections. Moreover, our primary aim in this work was to calculate the effect of the nuclear deformation on the binding energy, and hence other small effects were ignored consistently.

One interesting aspect of our results for the $1s$ single-particle energy has already been mentioned in Sec. IV, and it deserves some comments here. We have found that as the nucleon number increases the binding energy of this level increases much faster compared to those near the Fermi surface. This phenomenon has been noticed by earlier workers[17] also, and has been attributed to the nonlocality of the HF potential. There is some experimental evidence from $(e,e'\gamma)$ experiments[26] that the binding energy of this level really changes from ≈ 35 to 60 MeV as one goes from $A=12$ to 28. However, the interpretation of the data is not unambiguous in view of the very wide peak corresponding to the $1s$ level. More experimental investigations to settle this point conclusively seem to be necessary.

The HF determinant gives the zero-order intrinsic wave function of the nucleus. If the effects of the residual interactions are not strong enough, then the projected wave functions having good angular momentum correspond to actual states in the nucleus. For detailed spectroscopic calculations it becomes necessary to carry out this projection procedure. Up to the present time there is only one published work by Ripka *et al.*[8] that deals with this problem for the case of axially symmetric intrinsic deformation. Since the general method of calculating the intrinsic wave function through the HF procedure has been well established now, more and more spectroscopic calculations based on such wave functions are desirable.

In many cases there are two or more intrinsic HF wave functions which are fairly close to each other in energy. The lowest of such wave functions yield the ground state, when a suitable projection is made out of it. However, the states of same angular momentum may be projected out of the excited intrinsic wave functions also. In some nuclei the mixture of such states with each other may be quite important in fitting the spectroscopic details. One such case is fairly well known now, namely, the case of the ground and excited 0^+ states in O^{16}. The latter state belongs to a fairly low-

lying deformed intrinsic HF wave function. Brown[27] has dealt with this mixing without using HF wave functions. In a calculation using HF wave functions one encounters the following major difficulty. The intrinsic wave functions belong to different HF Hamiltonians, and hence are not orthogonal to each other. The states projected out of them are also not necessarily orthogonal. Hence there is a great deal of work involved in calculating the admixture and energies. Working out the details for such calculations will pave the way to many interesting applications.

Although HF calculations using realistic two-body potentials (like the present work) have already yielded encouraging results, it still remains to see whether these HF energies and wave functions lead to significantly different effective matrix elements at the next stage of a doubly self-consistent calculation. We therefore feel that such calculations be done in the future to put the HF method in the theory of nuclear structure on a firm foundation.

After the completion of this paper, we came to know that the matrix elements of the Yale potential used in this work are being revised by Shakin *et al.* A few of their new matrix elements differ from the old ones by about an MeV. Since these matrix elements are weighted by a lot of Moshinksy brackets and added together to give the two-nucleon matrix elements in the harmonic-osillator representation, we expect that this revision will not alter our results too much.

ACKNOWLEDGMENTS

We would like to thank Professor A. Kerman for suggesting the method of Lagrange multipliers and for helpful discussions, Professor Carl Shakin, Dr. Y. Waghmare, and Professor M. H. Hull for supplying the relative matrix elements for the Yale potential prior to publication, Dr. Juris Svenne for supplying his code to calculate the two-particle matrix elements, and Mrs. Katrina Stamp for assistance with the numerical calculations.

Finally we would like to express our thanks to Professor Herman Feshbach for extending the hospitality of the Laboratory for Nuclear Science at Massachusetts Institute of Technology.

APPENDIX I

Let us consider two t matrices with labels A and B, defined by equations similar to Eq. (8) of the main text. Bethe, Brandow, and Petschek[22] have derived the following general expression connecting two such t matrices:

$$t_A=t_B^\dagger+\Omega_B^\dagger(v_A-v_B)\Omega_A+t_B^\dagger\left[\left(\frac{Q_B^\dagger}{e_B}\right)-\frac{Q_A}{e_A}\right]t_A. \quad \text{(A1)}$$

[27] G. E. Brown and A. M. Green, Nucl. Phys. **75**, 401 (1966).

If only the potentials are different in the two cases, A and B, and the operators Q/e the same, then the equation simplifies to

$$t_A=t_B^\dagger+\Omega_B^\dagger(v_A-v_B)\Omega_A. \quad \text{(A2)}$$

The Møller wave operator Ω produces the perturbed wave function ψ operating on the unperturbed wave function ϕ. All other symbols have been defined in the main text.

We now identify the potential v_A as the entire two-body potential v, and resolve it into components that are diagonal (D) and nondiagonal (ND), respectively, in the relative orbital angular-momentum space. Only the tensor force (T) contributes to the latter component. We further break up the diagonal component into a long-range (l) and a short-range (s) part. We then identify the latter as v_B. Since t_A and Ω_A now correspond to the exact reaction and wave operators, we may omit the labels from them; we may further replace the label B by s (short range). Thus, Eq. (A2) yields

$$t=t_s^\dagger+\Omega_s^\dagger(v_{\mathrm{D}}{}^l+v_{\mathrm{ND}}{}^T)\Omega. \quad \text{(A3)}$$

If the hard core of the potential is followed by an attractive well (as in the $^3S_1$ state), then a separation distance d may be chosen for making the short- and long-range separation such that t_s has vanishing matrix elements for the relative two-body state under consideration. In such a case, Eq. (A3) states that the matrix element of t is the same as that of $(v_{\mathrm{D}}{}^l+v_{\mathrm{ND}}{}^T)$ evaluated between the wave function ψ_s (generated by Ω_s) corresponding to the short-range potential alone, and the exact wave function ψ (generated by Ω) corresponding to the entire two-body potential:

$$(\phi|t|\phi)=(\psi_s|(v_{\mathrm{D}}{}^l+v_{\mathrm{ND}}{}^T)|\psi). \quad \text{(A4)}$$

On the other hand, if the potential outside the hard core is repulsive (like in the $^3P_1$ state), then the above choice of a separation distance fails. In Shakin's work,[10] an attractive square-well pseudopotential, v_{sq} of adjustable radius d, has been introduced in such states to achieve the vanishing of the matrix elements of t_s. Then the matrix elements of t, of course, are equal to those of $(v_{\mathrm{D}}{}^l+v_{\mathrm{ND}}{}^T-v_{\mathrm{sq}})$ between the states mentioned above.

For practical calculations an expansion of ψ in terms of ψ_s is necessary. We have

$$\psi=\psi_s-(Q/e)(v_{\mathrm{D}}{}^l+v_{\mathrm{ND}}{}^T)\psi_s+\cdots. \quad \text{(A5)}$$

Using the first two terms of this expansion in (A4) one gets the expression of the t-matrix element derived in Shakin's work for the unitary-transformed effective matrix element. The present derivation shows that, in spite of the formal dissimilarities of the methods used, the introduction of the short-range and long-range separation in Shakin's work makes it completely identical with the t-matrix formalism. This is a consequence of the fact that the separation distance is

energy-dependent, and hence it spoils the unitarity of the transformation.

The most important contribution of $v_{\mathrm{ND}}{}^T$ in Eq. (A4), after the substitution of (A5), is given by

$$(\psi_s|v_{\mathrm{ND}}{}^T(Q/e)v_{\mathrm{ND}}{}^T|\psi_s),$$

where ψ_s refers to the relative ${}^3S_1$ state. Since $v_{\mathrm{ND}}{}^T$ is not included in the determination of the separation distance, the integration is to be performed carefully. Although ψ_s is zero inside the core there is a finite contribution to the above matrix element from the core because of the discontinuity in the gradient of ψ_s at the core radius. This is in addition to the contribution from core to infinity.

The core contribution has not been estimated in the work of Ref. 10. Furthermore, the occurence of the entire $v_{\mathrm{ND}}{}^T$, and the additional repulsive square-well $(-v_{\mathrm{sq}})$ in triplet odd states, ought to raise convergence questions that should be settled by higher-order calculations.

It is well known that other types of separation of the potential could also have been done in Eq. (A2). In the separation used by Kuo and Brown,[9] the nondiagonal component of the tensor force is explicitly included. These authors use the reference-spectrum method,[22] and not the separation method in triplet odd states. In both these respects, the Kuo-Born results should have better convergence.

In obtaining the separation distance from the equation satisfied by $t_s\phi$, the latter is usually simplified by substituting $(1/e_{\mathrm{H.O.}})$ for (Q/e). The $e_{\mathrm{H.O.}}$ denotes the energy denominator calculated with the harmonic-oscillator spectrum. Therefore, strictly speaking, the third term in (A1) should also be included as a correction term. It is given by

$$t_s{}^\dagger\left(\frac{1}{e_{\mathrm{H.O.}}}-\frac{Q}{e}\right)t$$

and can be separated into the so-called dispersion and Pauli corrections. The matrix elements calculated in Ref. 10 and used here, do not contain these corrections and the core contribution mentioned earlier.

APPENDIX II

In this appendix we shall derive the t-matrix equation to be solved in a fully self-consistent calculation. The matrix elements needed for setting up the HF equation are of the form $(rm|t|sm)$, where m is an occupied HF state and r, s may be both occupied and unoccupied states. (These nomenclatures are explained in Sec. I.) Each of these HF states are expressed in terms of harmonic-oscillator states, and then each pair of harmonic-oscillator states on the two sides of t can be expressed as a sum of products of relative and center-of-mass (c.m.) harmonic-oscillator states with the help of Moshinsky brackets.

The excited intermediate states used in the calculation of the t matrix can be very well approximated by plane-wave states $|k_1,k_2\rangle$, and hence the energy-denominator e can be written as

$$(\hbar^2/2M)(k_1{}^2+k_2{}^2)-\epsilon(s)-\epsilon(m)-\delta,$$

where $\delta=0$ when s is an occupied state, and it is a finite adjustable parameter when s is an unoccupied state. Since the intermediate states are well above the occupied states, the Pauli operator Q may be put equal to unity. Then, the t-matrix equation (8) of the text reduces to the following equation for the wave functions:

$$[-(\hbar^2/2M)(\nabla_1{}^2+\nabla_2{}^2)-\epsilon(s)-\epsilon(m)-\delta](\phi-\psi)=v\psi. \quad \text{(A6)}$$

We write

$$\nabla_1{}^2+\nabla_2{}^2=\nabla_R{}^2+\nabla_r{}^2,$$

where $\mathbf{R}$ and $\mathbf{r}$ are the c.m. and relative coordinates defined as

$$\mathbf{R}=\frac{1}{\sqrt{2}}(\mathbf{r}_1+\mathbf{r}_2), \quad \mathbf{r}=\frac{1}{\sqrt{2}}(\mathbf{r}_1-\mathbf{r}_2).$$

The reader should note that v is usually defined in terms of $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$, which differs from our definition by a numerical factor.

The operator $-(\hbar^2/2M)\nabla_R{}^2$ can now be approximated by its expectation value $\frac{1}{2}E_{NL}$ for the c.m. harmonic-oscillator state $|NL\rangle$. This approximation reduces (A6) to an equation for the relative coordinate only, which can be solved for the important relative angular-momentum states, namely the various S, P, D states. The solution of the differential equation, and the calculation of the relative t-matrix elements have been discussed by Kuo and Brown in Ref. 9. For our purpose the work has to be repeated for various values of E_{NL} and pair energies $\epsilon(s)+\epsilon(m)$.

Since Q has been substituted by unity in setting up Eq. (A6), it is a better approximation to use only a part of the potential up to a short distance d in this equation and solve it. The solution will yield a t_s (not necessarily zero). Then the corrections due to the long-range part of v can be calculated using (A1). This will reduce the Pauli correction.