HARTREE-FOCK CALCULATIONS
FOR LIGHT NUCLEI
(LECTURE NOTES)

M. BOUTEN

1968
MIRAMARE - TRIESTE
HARTREE-FOCK CALCULATIONS FOR LIGHT NUCLEI

(LECTURE NOTES)

M. Bouten *

TRIESTE
MAY 1968

* On leave of absence from C.E.N., Mol-Donk, Belgium
I. INTRODUCTION

The idea of doing a Hartree-Fock (HF) calculation for nuclei is suggested by the success of the nuclear shell model. In this model, the nucleons are assumed to move independently of each other in a potential well, at least in first order. In practical calculations, this well is chosen in a fairly arbitrary way containing several parameters which are then adjusted to reproduce good fits to the experimental data. For example, it is customary to choose a harmonic oscillator potential, the width of which is adjusted to the experimental radius and a one-body spin-orbit force, the strength of which is adjusted in order to obtain a best fit to the experimental energy spectrum. In this way, it is obvious that part of the success of the shell-model is obtained from the adjustable parameters. In a better theory, one should start from the nuclear Hamiltonian and calculate the shell-model potential from it. This is just what is done in atomic physics by means of the HF method. The reason why this method has not been taken over into nuclear physics up to recently is that the realistic interactions between nucleons contain an infinitely repulsive core. This implies that matrix elements of such an interaction between independently moving particles become infinite. In recent years some methods have been developed for eliminating the hard core. Also, some almost realistic interactions have been obtained which do not possess a hard core.

II. HF EQUATIONS

In the following we shall assume that a nucleon-nucleon interaction $V$ exists which is non-singular so that it may be used in HF calculations. We denote the Hamiltonian

$$ H = \sum_i T_i + \frac{1}{2} \sum_{i \neq j} V_{ij} $$

It is well known that the HF method is equivalent to finding a set of $A$ single-particle functions $u_\alpha (\lambda = 1, 2, \ldots, A)$
(called orbitals) such that the Slater determinant constructed with these functions

$$\phi = \det(u_1, u_2, \ldots, u_A)$$

makes the expectation value of the Hamiltonian minimum

$$\delta \frac{\langle \phi H \phi \rangle}{\langle \phi \phi \rangle} = 0$$  \hspace{1cm} (1)

If we use the labels $\lambda, \mu$ for occupied orbitals (i.e. contained in $\phi$) and $\sigma, \tau$ for unoccupied orbitals (i.e. not contained in $\phi$), then I remind you that the minimum condition (1) is equivalent to either of the following conditions 3):

1. **Brillouin condition**

$$\langle \phi H \phi^\sigma \rangle = 0 \hspace{1cm} \text{all } \lambda \leq A$$

$$\sigma > A$$  \hspace{1cm} (2)

where $\phi^\sigma = a_\sigma^+ a_\lambda \Phi$; $a_\lambda^+$ being a creation operator for a particle with orbital $u_\lambda$.

2. **HF condition**

$$\langle u_\alpha | h \{ u_1 \ldots u_A \} | u_\beta \rangle = \Sigma_\alpha \delta_{\alpha\beta} \hspace{1cm} \text{all } \alpha, \beta$$  \hspace{1cm} (3)

where $h\{ u_1 \ldots u_A \}$ is called the HF Hamiltonian. It is defined as

$$h = T + U\{ u_1 \ldots u_A \}$$

where $U$ is called the HF potential and is defined through its matrix elements between two arbitrary one-particle functions $| a \rangle$ and $| \lambda \rangle$ as
\[ \langle a | U | b \rangle = \sum_{\lambda=1}^{A} \langle a \, u_{\lambda} | V(1-P_{12}) | b \, u_{\lambda} \rangle \]  

where \( P_{12} \) is the permutation operator of particles 1 and 2. The notation \( \{ u_{1}, \ldots, u_{A} \} \) denotes the subspace of the one-particle Hilbert space spanned by the occupied orbitals \( u_{1}, u_{2}, \ldots, u_{A} \). It is clear from (4) that \( U \) depends only on this subspace and not on the particular basis chosen in it. The condition (3) is the usual form of the HF equations. They form a non-linear eigenvalue problem, the unknown orbitals \( u_{\lambda} \) coming also in the definition of the HF Hamiltonian \( h \). The \( u_{\lambda} \) must be eigenfunctions of the operator \( h \) which itself is constructed by means of the \( u_{\lambda} \). This is called the self-consistency condition.

III. SOLUTIONS OF THE HF EQUATION

The HF equations (3), being only a necessary condition for the minimum of the energy, have very many solutions. In fact it is easy to see that there is always an infinity of solutions of (3). The difficulty lies, however, in finding the solution which gives the lowest energy.

I shall first show that any set of plane waves with wave vectors \( \vec{k}_{1}, \vec{k}_{2}, \ldots, \vec{k}_{A} \) form a solution of (3). In the usual way, we take a large cube with periodic boundary conditions as normalization volume so that \( \langle \vec{k}_{i} | \vec{k}_{j} \rangle = \delta_{i,j} \). We show that

\[ \langle \vec{k}_{i} | h \{ \vec{k}_{1}, \vec{k}_{2}, \ldots, \vec{k}_{A} \} | \vec{k}_{j} \rangle = \epsilon_{i} \delta_{ij} \quad \text{all } i,j \]  

which will prove that \( \vec{k}_{1}, \vec{k}_{2}, \ldots, \vec{k}_{A} \) are a solution of (3). Using (4) we have for the l.h.s.

\[ \langle \vec{k}_{i} | T | \vec{k}_{j} \rangle + \sum_{\lambda=1}^{A} \langle \vec{k}_{i} \, \vec{k}_{\lambda} | V(1-P_{12}) | \vec{k}_{j} \, \vec{k}_{\lambda} \rangle \]

which equals
\[
\frac{\hbar^2 k_i^2}{2m} \delta_{ij} + \delta_{ij} \sum_{\lambda=1}^{A} \left< k_1^\lambda k_1^\lambda \left| V (1-P) \right| k_1^\lambda k_1^\lambda \right>
\]

because \( V \) commutes with the total momentum. This has the form of the r.h.s. of (5) with

\[
\epsilon_i = \frac{\hbar^2 k_i^2}{2m} + \sum_{\lambda=1}^{A} \left< k_1^\lambda k_1^\lambda \left| V (1-P) \right| k_1^\lambda k_1^\lambda \right>
\]

This proves that any set of \( A \) plane waves forms a solution of the HF equations (3). Since we are interested in finding the lowest solution (lowest total energy) we calculate the total energy

\[
\left< \phi H \phi \right> = \sum_{\lambda} \frac{\hbar^2 k_\lambda^2}{2m} + \frac{1}{2} \sum_{\lambda \neq \mu=1}^{A} \left< k_\lambda^\mu k_\mu^\lambda \left| V (1-P) \right| k_\lambda^\mu k_\mu^\lambda \right>
\]

Among all plane wave solutions, we then expect to find the lowest HF solution by taking the \( A \) plane waves with lowest kinetic energy. One usually assumes that this solution will also be the lowest solution among all HF solutions in the case of infinite systems like infinite nuclear matter. There is, however, no proof for this and OVERHAUSER 4) has shown that one may obtain a lower energy solution, also in the case of infinite systems, for special types of interactions.

In the case of finite nuclei, it seems obvious that the plane wave solution will not be the lowest one since the particles are interacting only very little, being smeared out over all space. How can we find a lower energy solution and especially the lowest one? In practical calculations, an iteration procedure is used to find a solution of the HF equations which you may hope will be the lowest one. One makes a guess for the occupied orbitals (call them \( u^{(1)}_\lambda \)), one calculates \( h \{ u^{(1)}_\lambda \} \) by means of (4) and diagonalizes it. Call its lowest \( A \) eigenfunctions \( u^{(2)}_1, u^{(2)}_2, \ldots, u^{(2)}_\Lambda \). Choosing these, one constructs \( h \{ u^{(2)}_\lambda \} \) by means of (4), diagonalizes again, chooses again its lowest \( A \) eigenfunctions and continues until self-consistency is obtained, i.e., until the \( u_\lambda \) in two consecutive steps of the iteration remain unchanged.
The reason for choosing the lowest eigenfunctions of \( h \{ u_\lambda \} \) at each step of the iteration is that one hopes that this set will give the lowest total energy \( \langle \phi H \phi \rangle \) at each step of the iteration. This is, however, not guaranteed because the total energy is not simply the sum of the single-particle \( \varepsilon_\lambda \)'s but one has

\[
\langle \phi H \phi \rangle = \sum_{\lambda=1}^{A} \varepsilon_\lambda - \frac{1}{2} \sum_{\lambda \neq \mu} \langle \lambda \mu \mid V (1-P) \mid \lambda \mu \rangle \quad (6)
\]

The iteration procedure described above is still a formidable work. In all practical calculations the problem has been simplified in either of two different ways:

1. Truncation of the one-particle Hilbert space

In most HF calculations for light nuclei, one has taken the subspace spanned by the lowest four harmonic oscillator shells \( 0s, 0p, 1s, 0d, 1p, 0f \). This is an eighty-dimensional subspace. If we call \( | i \rangle (i = 1, \ldots, 80) \) an orthonormal basis in this subspace, the HF orbitals \( u_\lambda \) are then determined by their expansion coefficients \( X^\lambda_i \).

\[
u_\lambda = \sum_{i=1}^{80} X^\lambda_i | i \rangle \quad (7)
\]

and the HF Hamiltonian \( h \{ u_\lambda \} \) is replaced by an eighty-dimensional matrix:

\[
\langle i \mid h \{ u_\lambda \} \mid j \rangle = \langle i \mid T \mid j \rangle + \sum_{\lambda=1}^{A} \sum_{k=1}^{80} \sum_{\ell=1}^{80} X^\lambda_k \langle ik \mid V (1-P) \mid j\ell \rangle X^\lambda_\ell \quad (8)
\]

The HF equations (3) are then replaced by the matrix equation:

\[
\sum_{j=1}^{80} \langle i \mid h \{ u_\lambda \} \mid j \rangle X^\lambda_j = \varepsilon_\lambda X^\lambda_i \quad (i = 1 \ldots 80) \quad (9)
\]

Thus the \( X^\lambda \) are the different eigenvectors of the matrix (8). One
again proceeds by iteration. Making an initial guess for the $A$ occupied eigenvectors (call them $X^{\lambda(1)}$), one calculates $\langle i | h^{(1)} | j \rangle$ by means of (8) and diagonalizes it. Calling the lowest $A$ eigenvectors $X^{\lambda(2)}$, one calculates again $\langle i | h^{(2)} | j \rangle$ by means of (8) and continues until self-consistency is obtained. This iteration procedure is obviously much simpler than the general iteration procedure sketched before, because diagonalizing a finite matrix is very much simpler than finding the lowest $A$ eigenfunctions of a general one-body operator.

If the dimension of the subspace is large, however, the numerical labour remains very large. For example, in the case of the finite eighty-dimensional space considered above, there are $\frac{80 \times 81}{2} = 3240$ matrix elements to be calculated at each step of the iteration. Each matrix element, calculated by means of (8), contains a sum of $A \times 80 \times 80 = 6400$ matrix elements of $V$. This large numerical problem can be simplified by the second approximation called the symmetry restriction.

2. Symmetry restriction

Suppose that our initial guess of the HF orbitals $u^{(1)}_\lambda$ has a certain symmetry. For definiteness let us suppose that each $u^{(1)}_\lambda$ has a definite parity; $I u^{(1)}_\lambda = \xi^{(1)}_\lambda u^{(1)}_\lambda$. Then the HF Hamiltonian constructed with the $u^{(1)}_\lambda$ will commute with the parity operator $[h \{ u^{(1)}_\lambda \}, I] = 0$. To show this, we only have to prove that $[U \{ u^{(1)} \}, I] = 0$. For general single-particle states $| a \rangle$ and $| b \rangle$, one has

$$\langle a | I^+ U I | b \rangle = \langle Ia | U | Ib \rangle$$

$$= \sum_{\lambda=1}^{A} \langle Ia, u^{(1)}_\lambda | V (1-P) | Ib, u^{(1)}_\lambda \rangle$$

from the definition of $U$. Transforming both bra and ket by the unitary operator $I$ gives (since $[I, V] = 0$)

$$= \sum_{\lambda=1}^{A} \langle a, I u^{(1)}_\lambda | V (1-P) | b, I u^{(1)}_\lambda \rangle$$

$$= \sum_{\lambda=1}^{A} |\xi^{(1)}_\lambda|^2 \langle a, u^{(1)}_\lambda | V (1-P) | b, u^{(1)}_\lambda \rangle = \langle a | U | b \rangle$$

-6-
Since \( |a\rangle \) and \( |b\rangle \) are general single-particle states, one has the operator relation

\[
I^+ U \{ u^{(1)}_\lambda \} I = U \{ u^{(1)}_\lambda \}
\]
or

\[
[ I, U \{ u^{(1)}_\lambda \} ] = 0
\]
The above proof only shows that if the probability density for finding the nucleons is symmetric for inversion through the origin, then the potential created by this mass distribution will also be symmetric.

Now, since \([ I, U \{ u^1 \} ] = 0\), the eigenfunctions of \( h \{ u^{(1)}_\lambda \} \) will have a definite parity

\[
I u^{(2)}_\lambda = \xi^{(2)}_\lambda u^{(2)}_\lambda
\]
In other words, the symmetry of the initial guess is conserved during the iteration and the iteration procedure will eventually converge to a solution having the same symmetry property. If the initial guess has a definite parity, the iteration procedure will always converge to a solution with a definite parity. A symmetry (like parity) which is conserved during the iteration procedure is called a consistent symmetry.

There are two aspects of consistent symmetries:

i) Starting from a guess with a definite parity, one will obtain a solution with a definite parity. This means that if the lowest HF solution does not have a definite parity (i.e. if the HF Hamiltonian has no inversion symmetry) one will never be able to obtain the lowest HF solution if one starts from a guess with a definite parity. If you want the lowest HF solution, you should start from a guess without symmetry.

ii) On the other hand, a consistent symmetry simplifies the numerical work considerably. Consider, for example, again the case of the eighty-dimensional subspace and take as basic states the oscillator functions,
An initial guess with a definite parity means that the \( u_{\lambda}^{(1)} \) (\( \lambda = 1,2,\ldots,A \)) have the following expansion:

\[
\begin{align*}
\text{either} \quad u_{\lambda}^{(1)} &= \sum_{i=1}^{28} X_{i}^{\lambda} |i\rangle + \text{parity} \\
\text{or} \quad u_{\lambda}^{(1)} &= \sum_{i=29}^{50} X_{i}^{\lambda} |i\rangle - \text{parity}
\end{align*}
\]

The matrix \( \langle i | h | j \rangle \{ u_{\lambda}^{(1)} \} \mid j \rangle \) reduces to the following form:

\[
\begin{array}{c|c|c}
28 & \text{\textcolor{white}{\textbullet}} & \text{\textcolor{white}{\textbullet}} \\
28 & \text{\textcolor{white}{\textbullet}} & \text{\textcolor{white}{\textbullet}} \\
28 & \text{\textcolor{white}{\textbullet}} & \text{\textcolor{white}{\textbullet}} \\
28 & \text{\textcolor{white}{\textbullet}} & \text{\textcolor{white}{\textbullet}} \\
\end{array}
\]

and each matrix element contains now at most \( A \times (52)^2 \) matrix elements of \( V \). Thus the simplification is threefold:

\[
\begin{align*}
- & \text{there are less matrix elements} \quad \langle i | h | j \rangle \\
- & \text{each matrix element contains less elements of } V \text{ in its sum} \\
- & \text{smaller matrices to diagonalize}
\end{align*}
\]

We shall see later that there is a fourth simplification if you have to make an angular momentum projection.

Thus, although one may lose the lowest solution of the HF equations by starting from a guess with a consistent symmetry, this has been done in all practical calculations in order to simplify the numerical labour.

Other consistent symmetries are axial symmetry (orbitals are eigenfunctions of \( j_z \)) and axial symmetry in isospace (orbitals are eigenfunctions of \( t_3 \)). To see how strongly these symmetries simplify the numerical work, let us consider again the above example. The orbitals are now eigenfunctions of \( I, j_z \) and \( t_3 \) with eigenvalues...
\[\pi, \gamma\] and \(\gamma\), respectively. The following table shows how many terms there are in their expansion in basic states:

<table>
<thead>
<tr>
<th>(\pi)</th>
<th>(\omega)</th>
<th>(\gamma)</th>
<th>number of terms in the expansion</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>(\pm \frac{5}{2})</td>
<td>(\pm \frac{1}{2})</td>
<td>1</td>
</tr>
<tr>
<td>+</td>
<td>(\pm \frac{3}{2})</td>
<td>(\pm \frac{1}{2})</td>
<td>2</td>
</tr>
<tr>
<td>+</td>
<td>(\pm \frac{1}{2})</td>
<td>(\pm \frac{1}{2})</td>
<td>4</td>
</tr>
<tr>
<td>-</td>
<td>(\pm \frac{7}{2})</td>
<td>(\pm \frac{1}{2})</td>
<td>1</td>
</tr>
<tr>
<td>-</td>
<td>(\pm \frac{5}{2})</td>
<td>(\pm \frac{1}{2})</td>
<td>2</td>
</tr>
<tr>
<td>-</td>
<td>(\pm \frac{3}{2})</td>
<td>(\pm \frac{1}{2})</td>
<td>4</td>
</tr>
<tr>
<td>-</td>
<td>(\pm \frac{1}{2})</td>
<td>(\pm \frac{1}{2})</td>
<td>6</td>
</tr>
</tbody>
</table>

Also, the matrix \(\langle i | h \{ u_\lambda \} | j \rangle\) is reduced very much. It contains along the diagonal

\[
\begin{cases}
4 \text{ submatrices of dimension 6} \\
8 \text{ " } 4 \\
8 \text{ " } 2 \\
8 \text{ " } 1
\end{cases}
\]

The total number of matrix elements \(\langle i | h | j \rangle\) which are non-zero has consequently decreased from 3240 to 196 and every matrix element itself is now a sum of at most \(A \times 36\) terms (instead of \(A \times 6400\)). The simplification in calculating the matrix \(\langle i | h | j \rangle\) is more than a factor 2000. You see how much you gain in numerical labour if you run the risk of losing the lowest solution. In many cases, however, one has found as lowest solution a solution having a higher symmetry than the symmetry of the initial guess and so you may hope that the symmetry restriction will not affect the accuracy of the method.

It is interesting now to know whether one can still further simplify the calculation by starting from a guess with a still larger
symmetry than the ones considered so far. Instead of talking about
the symmetry of the orbitals, it is somewhat easier to talk about the
symmetry of the HF Hamiltonian which is, of course, the same thing.
We have then seen that the assumption of axial symmetry, inversion
symmetry and \( t_3 \)-symmetry simplify the calculation considerably. May
we, for example, not assume that \( h \) be spherically symmetric? The
answer is: in some cases "yes", in most cases "no". Of course, we can
always start from an initial guess for \( h \), having spherical symmetry, but
the calculation is simplified only if the symmetry is conserved during
the iteration. Assume, for example, for a nucleus like \( ^5 \text{He} \), that \( h^{(1)} \)
be spherically symmetric. Its lowest eigenfunctions are then

- \( s \)-orbital : 4 times degenerate
- \( p \)-orbital : 12 times

So the next \( h^{(2)} \) will be constructed with four \( s \)-orbitals and one
\( p \)-orbital and cannot be any longer spherically symmetric. On the other
hand, for \( ^{16} \text{O} \) the next \( h^{(2)} \) will be constructed with four \( s \)-orbitals
and twelve \( p \)-orbitals and will again be spherically symmetric. Thus,
spherical symmetry is a consistent symmetry for \( ^{16} \text{O} \), but not for \( ^5 \text{He} \).
The question then is: for what nuclei will a certain group be a
consistent symmetry group? The answer to this question is not known
in general. One can, however, answer the inverse question (at least
partly): For what nuclei will a certain group not be a consistent
symmetry group? This will then exclude several symmetries as being
non-consistent for a given nucleus and one may try some of the
remaining groups and find out whether it is consistent or not by
doing the iteration.

The answer to the question: "For what \( A \)-values is a given
group \( G \) certainly not consistent symmetry group?" is based on the
following theorem:

If \( O \) is a unitary symmetry operator for the total Hamiltonian
\( H \) and if \( \{ u_1, u_2, \ldots, u_A \} \) is an invariant space under \( O \), then \( O \) is
also a symmetry operator for \( h \{ u_1, \ldots, u_A \} \). More formally,

\[
\text{if } [O,H] = 0, \quad \text{then } [O, h \{ u_\lambda \}] = 0
\]

\[
\text{if } O u_\lambda = \sum_{\mu=1}^{A} Q_{\lambda\mu} u_\mu \quad (\lambda = 1, \ldots, A)
\]

\[
\text{then } [O, h \{ u_\lambda \}] = 0
\]
The proof is exactly the same as that given previously for the
inversion operator \((C_{	ext{Ref.5}}\).

The theorem is also immediately extended to a group \(G\) of unitary
operators: if \([G,h]\) = 0 and if \(\{u_1 \ldots u_A\}\) is invariant under
all operators of \(G\), then \([G,h \{u_1 \ldots u_A\}] = 0\).

From the previous theorem there follows immediately the
trivial consequence that if \(G\) is a symmetry group for \(h\), it is
certainly necessary that there exists in the one-particle Hilbert
space a subspace of dimension \(A\) which is invariant under \(G\). In this
way, at least, one can start with an initial guess \(u^{(1)}\) having the
symmetry of the group \(G\). There is no guarantee that this symmetry
will be conserved during the iteration but, at least, those values
of \(A\) such that no invariant subspace of dimension \(A\) exists cannot
have \(G\) as a consistent symmetry group. One is thus led to study the
dimensions of the invariant subspaces in the one-particle Hilbert
space for the different groups \(G\). One finds, for example, for \(R_3\)
only even-dimensional subspaces and for the isospin group \(SU_2\) only a
two-dimensional subspace. If \(G\) is the product group \(R_3 \otimes SU_2\), the
invariant subspaces have dimensions which are multiples of four.
Thus for nuclei with \(A \neq 4n\), \(R_3 \otimes SU_2\) is certainly not a possible
symmetry group.

All this does not seem very useful. However, in the special
case of a group \(G\) for which all irreducible invariant subspaces
have the same dimension \(d\), then \(G\) is a consistent symmetry for all \(A\)
which are a multiple of \(d\). A trivial application of this are the
abelian groups considered previously \((I,j_z,t_3)\) which are consistent
symmetries for all values of \(A\). A non-trivial example is the two-
dimensional rotation reflection group which has only irreducible sub-
spaces of dimension two in the one-particle Hilbert space and the isospin
group \(SU_2\) which also has only two-dimensional irreducible subspaces.
As a result, the product of the two-dimensional rotation reflection
group and \(SU_2\) has only irreducible subspaces of dimension four and is
a consistent symmetry for \(A = 4n\). To show that the above statement
is true, let us start from an initial guess \(h^{(1)}\), commuting with \(G\).
It follows that the eigenvalues of \(h^{(1)}\) will have degeneracy \(d\), and
the \(A\) particles will just fill the lowest \(\frac{A}{d}\) levels. This space is
invariant under \(G\) and so \(h^{(2)}\) will commute with \(G\) from the above
theorem. Thus \(G\) is conserved as a symmetry group during the iteration
procedure and is thus a consistent symmetry.

For more details about these matters I refer to Ref. 5.

Most calculations so far have been done either for spherical nuclei \(^{160}\) \(^{40}\)Ca) where spherical symmetry is a consistent symmetry, or for \(Z = N = \) even nuclei \((A = 4n)\) for which the product of the two-dimensional rotation reflection group and \(SU_2\) is a consistent symmetry group. The reason, of course, is that this simplifies the numerical work very much. As stated above, you may lose the lowest HF solution. A typical example of this is \(^{12}\)C, for which spherical symmetry turns out to be consistent, but the resulting HF solution is not the lowest one. Starting from a guess without spherical symmetry, one finds a solution which is 14 MeV lower. 

IV. RESULTS OF HF CALCULATIONS

In this section, I want to describe a typical HF calculation for light nuclei. I am choosing the calculation which I think is the best one done so far. Many others have been done by other people, about which I will not talk, because I want to go on rather quickly to some HF calculations with angular momentum projection in the next lectures.

Kerman, Syvenne and Villars \(^7\) have made a HF calculation for the spherical nuclei \(^{160}\) and \(^{40}\)Ca using the TABAKIN interaction \(^2\). They have simplified the HF equations by assuming rotation inversion symmetry and charge independence and by expanding the orbitals in spherical oscillator functions. The occupied orbitals are thus written as

\[
\nu_\lambda = \sum_{n=0}^{N} X_\lambda^n | n \ell jm \rangle \tau \rangle 
\]

and they have truncated the space at \(N = 4\). The \(X_\lambda^n\) are the same for different orbitals corresponding to the same \(j\)-value.

Moreover, they optimize the total energy with respect to the oscillator parameter \(b\) by plotting the HF energy as a function of \(b\).

We describe their results for \(^{160}\) in some detail here. They find that the expansion coefficients \(X_\lambda^n\) decrease very rapidly with \(n\).
so that the truncation at \( N = 4 \) is justified. The single-particle spectrum \( \varepsilon_\lambda \) is shown below:

<table>
<thead>
<tr>
<th>( \varepsilon_\lambda )</th>
<th>( \varepsilon_\lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.74</td>
<td>0.93</td>
</tr>
<tr>
<td>6.12</td>
<td>2.09</td>
</tr>
<tr>
<td>2.31</td>
<td>-5.02</td>
</tr>
<tr>
<td>-9.45</td>
<td>-15.65</td>
</tr>
<tr>
<td>-19.65</td>
<td>-21.81</td>
</tr>
<tr>
<td>-48.72</td>
<td>-?</td>
</tr>
</tbody>
</table>

and the experimental single-particle energies \( \varepsilon_\lambda \) are given on the right. The comparison with experiment is based on the easily verified relation

\[
\varepsilon_\lambda = \langle \phi \Phi \rangle - \langle a^+_{\lambda \phi} | H | a^+_{\lambda \phi} \rangle \quad \lambda < \Lambda
\]

\[
\varepsilon_\sigma = \langle a^+_{\sigma \phi} | H | a^+_{\sigma \phi} \rangle - \langle \phi \Phi \rangle \quad \sigma > \Lambda \quad (11)
\]

where \( a^+_{\sigma \phi} | \phi \rangle \) and \( a^+_{\lambda \phi} | \phi \rangle \) are interpreted as states of \(^{17}O\) and \(^{15}O\) respectively. One sees that the lowest orbital is very deep, much deeper than is possible in a local potential which would have only three bound states. The comparison with the experimental single-particle energies is qualitatively good, but there are some discrepancies in the details. For example, the unoccupied orbitals \( d_{5/2} \) and \( s_{1/2} \) are not bound in contradiction with the experimental...
situation. We shall see that this comes out for many HF calculations and an explanation will be given further on.

The spin orbit splitting (e.g. between $d_{3/2}$ and $d_{5/2}$) is too large. A possible explanation of this was suggested by Elliott. He found that the spin orbit splitting is very sensitive to the size of the nucleus, the spin orbit splitting decreasing as the size increases. Kerman et al. did calculate the radius for $^{16}O$ and found it about 10% too small. Thus the too large spin orbit splitting may be related to the too small radius.

The total energy $\langle \phi | H | \phi \rangle = -38.5$ MeV compared to the experimental value $E_x = -127$ MeV. In order to improve the agreement, Kereman and Pal calculated the second-order correction to the total energy

$$\Delta E^{(2)} = \sum_{\lambda, \mu} \sum_{\sigma, \tau} \left| \frac{\langle u_\lambda u_\mu | V (1-P) | u_\sigma u_\tau \rangle}{E_\lambda + E_\mu - E_\sigma - E_\tau} \right|^2$$

occupied unocc.

They find

$$\Delta E^{(2)} \approx -69 \text{ MeV}$$

so that the total energy equals $-107.5$ MeV, which agrees satisfactorily with experiment. The fact that the second-order contribution is very large does not mean that the convergence of the perturbation theory is bad. In fact, one must compare $\Delta E^{(2)}$ with the first-order potential energy $\langle \phi | V | \phi \rangle$ which equals about $-350$ MeV and so

$$\frac{\Delta E^{(2)}}{\langle \phi | V | \phi \rangle} \leq 0.20$$

Bassichis, Kereman and Svenne extended these calculations to all $Z = N$ even nuclei with $A \leq 40$. They simplified the HF problem by:

i) Truncating the one-particle Hilbert space to the eighty-dimensional subspace spanned by the oscillator functions, $0s$, $0p$, $1s0d$, $1p$, $0f$.

ii) Restricting themselves to solutions with the symmetry of the two-dimensional rotation reflection group, good parity, time reversal and charge independence.
The occupied orbitals are thus written as

$$u_{\lambda} = \sum_{n\ell j} X_{n\ell j}^{\lambda} | n\ell j m, \tau > (-)^{\ell} \text{ fixed}$$

The $X_{n\ell j}^{\lambda}$ are real and are independent of $m$ and $\tau$ for fixed $n\ell j$.

The nuclei $^4\text{He}$, $^{16}\text{O}$ and $^{40}\text{Ca}$ are found to be spherical and will no more be discussed. The single-particle energies $\epsilon_{\lambda}$ for $^8\text{Be}$, $^{12}\text{C}$ and $^{20}\text{Ne}$ are shown below.
The levels below the dashed lines are the occupied ones. One finds a gap between occupied and unoccupied orbitals. This gap was discovered by Levinson in restricted HF calculations within the s-d shell, where it shows up much more clearly. In HF calculations, where all particles are taken into account, one also finds energy gaps between the "major shells" of the shell model and in the whole energy diagram; the Levinson gap is less conspicuous than in HF calculations within one major shell.

As in the case of $^{16}O$, it is again found that the unoccupied orbitals in $^8Be$ and $^{12}C$ have a positive single-particle energy, in contradiction to experimental bound nuclei $^9Be$ and $^{13}C$ and the single-particle $3/2^+$ state in $^{20}Ne$ is only just bound, compared to a well bound $^{21}Ne$ nucleus. The explanation of this discrepancy is probably the following. It is known from Levinson's work that the gap between occupied and unoccupied orbitals is considerably larger for $Z = N = \text{even nuclei (}^8Be, ^{12}C, ^{16}O, ^{20}Ne\text{)}$ than for the neighbouring odd nuclei. So it is to be expected that configuration admixtures will be more important for the odd nuclei, resulting in a larger correlation energy which will make the odd nuclei bound.

Bassichis et al. finds the following values for the expansion coefficients of the orbitals:

$\hat{E}_c$: 

\begin{align*}
\langle \frac{1}{2}^+ \rangle &= -0.96 \left| os \frac{1}{2} \right> -0.20 \left| od \frac{5}{2} \right> -0.02 \left| ls \frac{1}{2} \right> +0.18 \left| od \frac{3}{2} \right> \\
\langle \frac{1}{2}^- \rangle &= 0.85 \left| op \frac{3}{2} \right> -0.50 \left| op \frac{1}{2} \right> +0.13 \left| of \frac{7}{2} \right> -0.01 \left| lp \frac{3}{2} \right> \\
&\quad\quad\quad-0.11 \left| of \frac{5}{2} \right> +0.03 \left| lp \frac{1}{2} \right>
\end{align*}

It is interesting to rewrite these in a L-S coupling basis 
\[ |n l \ell_m \rangle \] . This becomes

\begin{align*}
\langle \frac{1}{2}^+ \rangle &= -0.96 \left| os \frac{1}{2} \right> -0.27 \left| od \frac{1}{2} \right> +0.013 \left| od \frac{3}{2} \right> -0.02 \left| ls \frac{1}{2} \right> \\
\langle \frac{1}{2}^- \rangle &= 0.98 \left| op \frac{1}{2} \right> +0.08 \left| op \frac{3}{2} \right> + \ldots \ldots \\
\end{align*}
The remarkable thing is that \( u(\frac{1}{2}+) \) and \( u(\frac{1}{2}-) \) are to a very good approximation eigenfunctions of \( \hat{J}_z \) with eigenvalue zero. This is just what one obtains if one makes a HF calculation starting from a central interaction. We see that spin orbit and tensor forces play a very negligible role in determining the HF orbitals for \( \text{Be} \).

If you do the same thing for \( ^{12}\text{C} \) and for \( ^{20}\text{Ne} \), you find

\[
^{12}\text{C}: \\
u(\frac{3}{2}^-) = 0.99 | 0\psi\frac{1}{2} > + \ldots \ldots \\
u(\frac{1}{2}^-) = -0.98 | 0\psi\frac{1}{2} > -0.18 | 0\psi\frac{1}{2} > + \ldots \ldots \\
^{20}\text{Ne}: \\
u(\frac{1}{2}^+) = 0.03 | 0s\frac{1}{2} > -0.86 | 0d\frac{1}{2} > -0.30 | 0d\frac{1}{2} > + 0.40 | 1s\frac{1}{2} >
\]

So you again find that \( \psi \) are approximately eigenfunction of \( \hat{J}_z \) for \( ^{12}\text{C} \) but with a larger admixture of different \( \hat{J}_z \) values and for \( ^{20}\text{Ne} \) this is still worse. Spin orbit and tensor forces become more and more effective in determining the HF orbitals as one goes to heavier nuclei. For light nuclei, as \( \text{Be} \), they can be neglected.

The total energies \( \langle \phi | H | \phi \rangle \) obtained by Bassichis et al. again deviate strongly from the experimental energies. However, since the nuclei turn out to be deformed (except for \( ^4\text{He}, \text{Ca} \)), \( \phi \) is not an eigenfunction of the total angular momentum \( J \) and can consequently not be associated with a particular physical state. One can, however, develop \( \phi \) in eigenstates of \( J^2 \).

\[
\phi = \sum_J \psi_j
\]

and associate \( \psi_j \) with the lowest physical state with angular momentum \( J \). The energy for this state is then \( E_j = \langle \psi_j | H | \psi_j \rangle \).

In order to calculate \( E_j \) from a knowledge of \( \langle \phi | H | \phi \rangle \), Bassichis et al. postulates that the \( E_j \) are related as in a rotational band

\[
E_j = E_0 + B J(J+1)
\]

One then has
Calculating both $\langle \phi H \phi \rangle$ and $\langle \phi J^2 \phi \rangle$, one can obtain $E_0$ if one knows $B$. Theoretical methods for calculating $B$ are very unsuccessful. Therefore Bassichis et al. have taken $B$ from the experimental knowledge of the lowest excited $2^+$ state. They get, e.g., for $^{20}\text{Ne}$

\[
\begin{align*}
\langle \phi H \phi \rangle &= -51.8 \text{ MeV} \\
E_0 &= -56.0 \text{ MeV} \\
E_x &= -179.2 \text{ MeV}
\end{align*}
\]

In the same way as for $^{16}\text{O}$, they calculate the second-order correction $\Delta E^{(2)}$ for the energy by means of (12). In this way, the agreement with experiment is improved a lot. E.g., for $^{20}\text{Ne}$, they find

\[
E_0 + \Delta E^{(2)} = -150.5 \text{ MeV}
\]

There seems, however, to be no justification for using the standard perturbation theory formula (12) for deformed nuclei. For $^{16}\text{O}$, the HF determinant $\phi$ can be considered as an approximation to the exact eigenfunction of $H$. Splitting $H$ into

\[
H = \sum_i h(i) + \left\{ \frac{1}{2} \sum_{i \not= j} V_{ij} - \sum_i U(i) \right\}
\]

where $h(i)$ is the HF Hamiltonian, one can use standard perturbation theory. In the case of deformed nuclei, $\phi$ is a very bad approximation for the real eigenstates of $H$, but $\psi_J$ is probably a good approximation. However, whereas $\phi$ is an eigenfunction of $\sum_i h(i)$, $\psi_J$ is not.

So using $\psi_J$ as an approximation for the real states, one should split up the total Hamiltonian $H$ in a different way:

\[
H = H_0 + H_1
\]

where $H_0 \psi_J = E_J \psi_J$. It is, however, not easy to find a simple expression for $H_0$. 

\(16\)
Another quantity which is calculated is the intrinsic quadrupole moment

\[ Q_{\text{intr}} = \langle \phi | Q_{20} | \phi \rangle \]  

(17)

The sign of \( Q_{\text{intr}} \) indicates whether \( \phi \) is prolate or oblate. Bassichis et al. found that only \( ^{12}\text{C} \) and \( ^{28}\text{Si} \) are oblate; all the other nuclei are prolate. In order to compare with experimental quadrupole moments or \( B(E2) \)'s, one has to postulate some relation between \( Q_{\text{intr}} \) and observable quantities (in the same way as for the energies \( E_j \)). If we postulate the rotational model relation

\[ B(E2; 2 \rightarrow 0) = \frac{1}{16\pi} | Q_{\text{intr}} |^2 \]  

(18)

one finds, e.g., for \( ^{12}\text{C} \), \( B(E2; 2 \rightarrow 0) = 5.2 \text{ fm}^4 \), compared to the experimental value \( 8.4 \text{ fm}^4 \). We have already remarked above that the calculated radii are about 10% too small. A larger radius will obviously increase \( Q_{\text{intr}} \) and consequently also \( B(E2; 2 \rightarrow 0) \) giving a better fit to the experimental result.

In the next section, I will show how you can calculate with the function \( V_j \) directly without having to postulate some relations between intrinsic and observable quantities which are not very well satisfied for light nuclei.

To conclude this section, I want to compare some properties of the HF potential with what one expects about it from standard shell-model calculations. Kurath's intermediate coupling calculation in the \( p \)-shell used a shell-model potential

\[ U_{\text{STM}} = U_{\text{oscillat}} + \xi \vec{L} \cdot \vec{S} \]

Treating \( \xi \) as an adjustable parameter, Kurath found best fits to the experimental spectra if \( \xi \) increased through the shell. In the \( s-d \) shell also, a larger spin orbit splitting is needed at the end of the shell than at the beginning. Let us see if this comes out here.

\[ ^{16}\text{O} : \quad d_2^3 - d_2^5 = 8.4 \text{ MeV} \]

\[ ^{40}\text{Ca} : \quad d_2^3 - d_2^5 = 13.3 \text{ MeV} \]
Another property of shell-model potential in the s-d shell is the so-called s-d inversion. In $^{17}$O, the s-orbital is known to lie below the centre of gravity of the d-orbitals whereas in $^{39}$Ca the s-orbital is lying above. In the HF calculation, the s-orbital lies above the centre of gravity of the d-orbitals both in $^{16}$O and $^{40}$Ca, so the inversion is not found. It is maybe interesting to remark that BARANGER and MUTHUKrishna $^{12}$ did find the s-d inversion in a HF calculation using the central Yamaguchi potential.

V. PROJECTION OPERATORS

In general, the HF determinant $\phi$ is not an eigenfunction of $J^2$ and cannot be interpreted as an approximate description of a particular physical state. In this case, it is usual to look on $\phi$ as an "intrinsic state" in the same sense as in the Nilsson model. Insofar as this intrinsic state is sufficiently stable, the real physical states are then associated with different rotational states of the intrinsic state $\phi$. The way to obtain wave functions for these rotational states from a knowledge of $\phi$ is not well known. The best way so far seems to be by means of projection operators for the angular momentum. For simplicity I will assume in this section that $\phi$ is already an eigenfunction of $J_z$ with eigenvalue $K$:

$$J_z \phi = K \phi$$  (19)

(this is so if the HF potential is axially symmetric). Expanding $\phi$ in eigenfunctions of $J^2$

$$\phi = \sum_j \psi_{jK}$$  (20)

one can obtain the function $\psi_{jK}$ from $\phi$ by means of a projection operator $P_J$

$$\psi_{jK} = P_J \phi$$  (21)

An expression of $P_J$ is, for example,

$$P_{J^p} = \frac{1}{(2J+1)(2J-1)} \left\{ \frac{J^2 - J_1 (J_1 + 2)}{J_p(J_p+1) - J_1(J_1+1)} \right\}$$  (22)
where $\mathbf{J}^2$ is the quantum mechanical operator for the total angular momentum. That is, $P_j$ is an infinite product of operators, one for each value of $J_i = 0,1,2, \ldots$, with the exception of $p$. The expression (22) is, however, in general very difficult to work with. A more useful expression for $P_j$ is based on some properties of the rotation matrices

$$ P_j = \frac{2j+1}{8\pi^2} \int \mathcal{O} \ \mathcal{D}_j^*(\Omega) \ R_\Omega $$

(23)

Here $\Omega$ is a shorthand notation for the three Euler angles; $\Omega = (\phi \theta \psi)$ and

$$ \int d\Omega = \int d\phi \int_0^\pi d\theta \int_0^{2\pi} d\psi $$

(24)

The operator $R_\Omega$ is the rotation operator

$$ R_\Omega = e^{-i\phi J_z} e^{-i\theta J_y} e^{-i\psi J_z} $$

(25)

and the function $\mathcal{D}_j^j(\Omega)$ are the representation matrices

$$ \mathcal{D}_j^j(\Omega) = \langle J K | R_\Omega | J K' \rangle = e^{-iK\psi} \mathcal{D}_j^j(\phi) e^{-iK'\psi} $$

(26)

It is easily seen, using standard properties of the D-functions, that the operator $P_j$ defined by (23) is a projection operator for the angular momentum $j$. The operator $P_j$ is a hermitian projection operator which means that

$$ P_j^+ = P_j $$

$$ P_j^2 = P_j $$

Useful operators are the related operators

$$ P_{Jj} = \frac{2j+1}{8\pi^2} \int \mathcal{O} \ \mathcal{D}_j^j(\Omega) \ R_\Omega $$

(27)

which construct the "partner-functions" $\psi_{Jj}$ of $\psi_{JK}$. The operators $P_{Jj}$ are, however, neither hermitian nor projection operators.
The energy $E_J$ corresponding to the projected state $\psi_{JK}$ can now be expressed as follows, using the fact that the Hamiltonian is a scalar, or

$$[H, P_J] = 0$$

One has

$$E_J = \frac{\langle \psi_J | H | \psi_J \rangle}{\langle \psi_J | \psi_J \rangle} = \frac{\langle \phi | H | P_J \phi \rangle}{\langle \phi | P_J | \phi \rangle}$$

$$= \frac{\int D_{KK}^J(\Omega) \langle \phi | H R_\Omega \phi \rangle d\Omega}{\int D_{KK}^J(\Omega) \langle \phi | R_\Omega \phi \rangle d\Omega}$$

(29)

Using (19) and (26) one can easily carry out the integration over $\psi$ and $\psi$ (this is the advantage of assuming (19)), so that

$$E_J = \frac{\int_0^{\pi} \sin^2 \theta d\theta d_{KK}^J(\theta) h(\theta)}{\int_0^{\pi} \sin^2 \theta d\theta d_{KK}^J(\theta) n(\theta)}$$

where

$$h(\theta) = \langle \phi | H e^{-i\theta J_\theta} \phi \rangle$$

$$n(\theta) = \langle \phi | e^{-i\theta J_\theta} \phi \rangle$$

(31)

Before describing how the functions $h(\theta)$ and $n(\theta)$ can be calculated, I want to make some remarks about the interpretation of the functions $P_J \phi$ as rotational states. Peterls and Yugo 13 introduced the projection operators as a quantum mechanical description of the rotation of the intrinsic state $\phi$. They put
themselves the following problem. Since \([H, R_{\Omega}] = 0\), it means that

\[ \langle \phi H \phi \rangle = \langle R_{\Omega} \phi | H | R_{\Omega} \phi \rangle \]

for all \( \Omega \). So let us try to find the best superposition of these "degenerate functions" \( R_{\Omega} \phi \)

\[ \psi = \int f(\Omega) R_{\Omega} \phi \; d\Omega \]

in the sense that

\[ \delta \frac{\langle \psi H \psi \rangle}{\langle \psi \psi \rangle} = 0 \]

The answer to this problem is

\[ f(\Omega) = D_{MK}^{J} (\Omega) \quad (32) \]

The function \( \psi \) is a superposition of the intrinsic function \( \phi \) rotated over different angles \( \Omega \). To see that it may correspond to a rotational state, consider the case that \( \phi \) is very strongly deformed so that both \( n(\theta) \) and \( h(\theta) \) go rapidly to zero as \( \theta \) increases. In this case we can approximate the \( d_{KK}^{J} (\theta) \) function in (30) by the first term of its Taylor expansion

\[ d_{KK}^{J} (\theta) \approx 1 - \frac{\theta^2}{4} \left[ J(J + 1) - K^2 \right] + \ldots. \quad (33) \]

This expression can easily be obtained from the defining equation (26) by expanding the exponential

\[ d_{KK}^{J} (\theta) = \langle J K | e^{-i\theta J_y} | J K \rangle \]

\[ \approx \langle J K | 1 - \frac{\theta^2}{2} J_y^2 | J K \rangle \]

\[ = 1 - \frac{\theta^2}{2} \left< J K \left| \frac{J_x^2 + J_y^2}{2} \right| J K \right> \]

\[ = 1 - \frac{\theta^2}{4} \left< J K \left| J_x^2 - J_z^2 \right| J K \right> \quad (34) \]
where we have used the obvious relations

\[ \langle J K | J_y | J K \rangle = 0 \] (35)

\[ \langle J K | J_x^2 | J K \rangle = \langle J K | J_y^2 | J K \rangle \] (36)

Introducing (33) into (30) one obtains

\[ E_J \approx \frac{\int h(\theta) \sin \theta \, d\theta - \frac{1}{4} [J(J+1) - K^2] \int \sin \theta \, d\theta \, \theta^2 h(\theta)}{\int n(\theta) \sin \theta \, d\theta - \frac{1}{4} [J(J+1) - K^2] \int \sin \theta \, d\theta \, n(\theta)} \] (37)

Since the second term, both in the numerator and the denominator, is small compared to the first term (from the assumption for \( n(\theta) \) and \( h(\theta) \)) one has

\[ E_J \approx \frac{\int h(\theta)}{\int n(\theta)} + \frac{1}{4} [J(J+1) - K^2] \frac{\int h(\theta) \int \theta^2 h(\theta) - \int \theta^2 h(\theta) \int n(\theta)}{[\int n(\theta)]^2} \] (38)

where we used the notation

\[ \int f(\theta) \equiv \int \sin \theta \, d\theta \, f(\theta) \]

Thus, the energies \( E_J \) are related as in the rotational model

\[ E_J = A + B [J(J+1) - K^2] + \ldots \]

In the same limit of strong deformation, one also finds that the same relations are valid between \( B(E2) \) values and the "intrinsic quadrupole moment" \( Q_{\text{int}} \) as in the rotational model. One is then justified in saying that the functions \( P_J \phi \) correspond to rotational states of the intrinsic state \( \phi \). This is in fact not surprising because, if \( \phi \) is strongly deformed, it defines a
direction in space and this is, from the uncertainty principle, only possible if \( \phi \) contains very many angular momentum states which are related among themselves as having the same internal structure, or, in other words, only if \( \phi \) contains a "rotational band". Projecting out states with a definite \( J \) will then produce the rotational states which are contained in \( \phi \). On the other hand, if \( \phi \) does not contain rotational states, \( P_J \) will still project states with definite \( J \) but the wave functions \( P_J \phi \) will not be related as rotational states. The operator \( P_J \) has nothing to do with "rotating the system \( \phi \)", but if \( \Phi \) contains a rotational band, \( P_J \) will project the rotational states out.

A simple example showing clearly that a state \( P_J \phi \) cannot mean a rotational state of the intrinsic state \( \phi \), is given by the LS-coupling shell-model wave functions for \( ^6 \)Li. In the shell model one takes the configuration \((\text{os})^4 (\text{op})^2 \) which for the most symmetric partition \([4,2]\) can couple to \( L = 0 \) and \( L = 2 \). These shell-model functions can be written as L-projections from an "intrinsic state" \( \phi' \), which can be taken as a simple Slater determinant

\[
\phi' = \det \left| \begin{array}{c}
(0s)^n (0p0)^{n+} (0p0)^{n+}
\end{array} \right|
\]

One has

\[
\psi_L = 0 = P_L = 0 \phi',
\psi_L = 2 = P_L = 2 \phi'
\]

One easily calculates \( \langle \phi Q_{20} \phi' \rangle = \frac{2\sqrt{5}}{\sqrt{\pi}} b^2 \) where \( b \) is the oscillator length parameter. Thus \( \phi' \) is a prolate state and one might be inclined to say that \( \psi_{L=0} \) and \( \psi_{L=2} \) correspond to rotations of a cigar-shaped \( ^6 \)Li. However, these same LS-coupling wave functions can also be written as

\[
\psi_L = 0 = P_L = 0 \phi',
\psi_L = 2 = P_L = 2 \phi'
\]

where \( \phi' \) is another Slater determinant.
\[ \phi' = \left| (0s)^{\alpha} (0p)^{n+} (0p-1)^{p+} \right| \]

and one easily calculates \[ \langle \phi' | \mathcal{Q}_{20} | \phi' \rangle = -\frac{\sqrt{5}}{\sqrt{4\pi}} b^2 \]

so that \( \mathcal{V}_{L=0} \) and \( \mathcal{V}_{L=2} \) could just as well be interpreted as "rotational states of a pancake-shaped \( ^6\text{Li} \).

In fact, any wave function with a definite \( J \) can always be written as a \( J \)-projection from an infinite number of different intrinsic states. It is only possible to talk about rotational states if you have a large set of functions with different \( J \)-values, which are related among themselves as in the rotational model and an equivalent way of saying this is that they all can be obtained by angular momentum projection from a strongly deformed intrinsic state.

Let us now return to formula (31) and see how \( h(\theta) \) and \( n(\theta) \) can be calculated. If these functions are known, a simple integration yields the projected energies \( E_j \).

1. Approximate method

In the case of strongly deformed \( \phi \), the functions \( n(\theta) \) and \( h(\theta) \) go rapidly to zero as \( \theta \) increases. For small values of \( \theta \), one has

\[ n(\theta) \approx \langle \phi | 1 - \frac{\theta^2}{2} J_y^2 | \phi \rangle \]

\[ h(\theta) \approx \langle \phi | H \left( 1 - \frac{\theta^2}{2} J_y^2 \right) | \phi \rangle \]

up to third order in \( \theta \).

An expression for \( n(\theta) \) and \( h(\theta) \) which is correct for small values of \( \theta \) and which goes rapidly to zero as \( \theta \) increases is

\[ n(\theta) = \exp \left[ -\frac{\theta^2}{2} \langle \phi | J_y^2 | \phi \rangle \right] \]

\[ h(\theta) = \langle \phi | H | \phi \rangle \exp \left[ -\frac{\theta^2}{2} \frac{\langle \phi | J_y^2 | \phi \rangle}{\langle \phi | H | \phi \rangle} \right] \]

(39)
LAMME and BOEKER \(^{14}\) have tested this approximation for light nuclei \(^{8}\)Be, \(^{12}\)C, \(^{16}\)O. They find that the energies calculated by using these approximate expressions differ from the exact results only by a few percent. As is to be expected, they find that the agreement improves as \(\phi\) becomes more deformed.

VERHAER \(^{15}\) has remarked that in the case \(K = 0\), the functions \(n(\theta)\) and \(h(\theta)\) may become large again for \(\theta = \pi\). This method can easily be adapted to include this case.

2. Exact method

Let us first consider how to calculate \(n(\theta) = \langle \phi \mid e^{-i\theta j_y} \mid \phi \rangle\) where \(\phi\) is the normalized Slater determinant

\[
\phi = \frac{1}{\sqrt{A!}} \det [u_1 \ u_2 \ldots \ u_A]
\]

Then \(e^{-i\theta j_y} \tilde{\phi}\) is also a Slater determinant which we denote with a bar above \(\phi\). We write

\[
\bar{\phi} = \frac{1}{\sqrt{A!}} \det [\bar{u}_1 \ \bar{u}_2 \ldots \ \bar{u}_A]
\]

where \(\bar{u}_\lambda = e^{-i\theta j_y} u_\lambda\). So \(n(\theta)\) is the overlap of the two Slater determinants \(\phi\) and \(\bar{\phi}\). It is well known \(^{16}\) that this equals the determinant of the overlap matrix \(O\) defined by its matrix elements

\[
O_{\lambda \mu} = \langle u_\lambda | \bar{u}_\mu \rangle = \langle u_\lambda | e^{-i\theta j_y} | u_\mu \rangle \quad (40)
\]

Thus

\[
\kappa(\theta) = \det O \quad (41)
\]

In order to calculate the matrix elements \(O_{\lambda \mu}\), one expands the orbitals \(u_\lambda\) and \(u_\mu\) in eigenfunctions of \(j^2\) (this is just the form in which the orbitals are obtained in actual HF calculations).
\[ u_\lambda = \sum_i X_i^\lambda |i\, j_1\, m_\lambda \rangle \]
\[ u_\mu = \sum_i X_i^\mu |i\, j_1\, m_\mu \rangle \]

(42)

where \( m_\lambda \) and \( m_\mu \) are fixed, since we are considering only the case of axial symmetry here. (Extension to non-axially symmetric HF solutions is straightforward, but more tedious.) One immediately obtains

\[ O_{\lambda\mu} = \sum_i \sum_{i'} X_i^\lambda X_{i'}^\mu \delta_{m_\lambda, m_\mu} \delta_{j_1, j_1'} \]

(43)

This is simple to calculate if the number of terms in the sum is small. Introducing these functions in the overlap matrix \( O \), it is easy to calculate the determinant of \( O \) if either \( \lambda \) is very small or if the matrix \( O \) is reduced to a simple form. The latter happens if the orbitals \( u_\lambda \) have some symmetry, commuting with the rotation operators. At this stage then, you see how the symmetry restriction described in Sec. 3 also simplifies the calculation of \( n(\theta) \) and consequently of the angular momentum projection. The symmetry restriction has a consequence that the number of terms in the expansion (42) is much smaller and consequently simplifies the calculation of \( O_{\lambda\mu} \).

On the other hand, the symmetry restriction also has as a consequence a reduction of the matrix \( O \). To illustrate how simple the calculation of \( n(\theta) \) may become in special cases, I consider again the LS-coupling shell-model wave function of \( ^6\text{Li} \) already considered above. In this case

\[ \phi = \frac{1}{\sqrt{6!}} \det \left| (os)^{n^+} (os)^{n^-} (os)^{p^+} (os)^{p^-} (opo)^{n^+} (opo)^{p^+} \right| \]

where the superscripts \( n^+, p^- \), etc., describe the spin-isospin quantum numbers, neutron with spin \( \frac{1}{2} \), proton with spin \( \frac{1}{2} \), etc. Since we consider an \( L \)-projection here (and not a \( J \)-projection) the overlap matrix \( O \) is defined as

\[ O_{\lambda\mu} = \langle u_\lambda | e^{-i\theta J_x} | u_\mu \rangle \]

-28-
This gives

\[
O = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & \cos \theta
\end{bmatrix}
\]

i.e. a diagonal matrix, due to the symmetry of the orbitals (which are eigenfunctions of I, \(s_z\) and \(t_3\)). We have used the special expressions for d-functions

\[
d_{oo}^0(\theta) = 1 \\
d_{oo}^1(\theta) = \cos \theta
\]

It follows that

\[
h(\theta) = \det O = \cos^2 \theta
\]

In order to calculate \(h(\theta)\) we must calculate matrix elements of both one-body and two-body operators between \(\phi\) and \(\overline{\phi}\).

\[
h(\theta) = t(\theta) + v(\theta)
\]

where

\[
t(\theta) = \langle \phi | \sum_i T_i | \overline{\phi} \rangle
\]

\[
v(\theta) = \langle \phi | \frac{1}{2} \sum_{i\neq j} V_{ij} | \overline{\phi} \rangle
\]

We first consider the one-body operator part \(t(\theta)\). One has, due to the antisymmetry of the Slater determinants
\[ \langle \phi | \sum_i T_i | \bar{\phi} \rangle = A \langle \phi | T_1 | \bar{\phi} \rangle \] (46)

Expanding \( \phi \) and \( \bar{\phi} \) in the first particle

\[
\phi = \frac{1}{\sqrt{A}} \sum_{\lambda=1}^{A} (-)^{\lambda+1} u_\lambda \phi_\lambda (2 \ldots A)
\]

\[
\bar{\phi} = \frac{1}{\sqrt{A}} \sum_{\lambda=1}^{A} (-)^{\lambda+1} \bar{u}_\lambda \bar{\phi}_\lambda (2 \ldots A)
\]

where

\[
\phi_\lambda (2 \ldots A) = \frac{1}{\sqrt{(A-1)!}} \det \begin{vmatrix} u_1 & u_2 & \ldots & u_{\lambda-1} & u_{\lambda+1} & \ldots & u_A \end{vmatrix}
\]

and introducing this into (45), we get

\[
\langle \phi | \sum_i T_i | \bar{\phi} \rangle = \sum_{\lambda, \mu=1}^{A} (-)^{\lambda+\mu} \langle u_\lambda | T | \bar{u}_\mu \rangle \langle \phi_\lambda | \bar{\phi}_\mu \rangle
\] (47)

Now \( \langle \phi_\lambda | \bar{\phi}_\mu \rangle \) is again equal to the determinant of the overlap matrix corresponding to the orbitals of \( \phi_\lambda \) and \( \bar{\phi}_\mu \). This is just the submatrix of \( O \) obtained by erasing the row \( \lambda \) and the column \( \mu \). This is easily calculated in the same way as \( n(\theta) \). The matrix element \( \langle u_\lambda | T | \bar{u}_\mu \rangle \) is further calculated by introducing the expansion (42) yielding

\[
\langle u_\lambda | T | \bar{u}_\mu \rangle = \sum_{i} \sum_{i'} X_i^\lambda X_{i'}^\mu \langle \lambda_{i_i} m_\lambda | T | i_{i'_i} m_\mu \rangle \delta_{i_i i'_i} \times d_{m_\lambda m_\mu} (\theta)
\] (48)

which again is quite simple if the number of terms in the expansion (42) is small. In the above example of \( ^6 \)Li one obtains in this way (because \( O \) is diagonal)

\[
\langle \phi | \sum_i T_i | \bar{\phi} \rangle = \sum_{\lambda} (u_\lambda | T | \bar{u}_\lambda) (\phi_\lambda | \bar{\phi}_\lambda)
\]

\[
= 4 (\cos^2 \theta + 2 \cos^2 \theta) = 30
\]
For the two-body part $\Psi(\theta)$ one proceeds exactly in the same way, expanding $\phi$ and $\overline{\phi}$ in determinants of particle 1 and 2. This gives

$$
\langle \phi | \sum_{i=j}^{2} V_{ij} | \overline{\phi} \rangle = \sum_{\lambda<\mu \nu<\rho} (-)^{\lambda+\mu+\nu+\rho} (u_{\lambda} u_{\mu} V(1-P) u_{\nu} u_{\rho})
$$

$$
(\phi_{\lambda\mu} | \phi_{\nu\rho})
$$

(49)

where

$$
\phi_{\lambda\mu} = \frac{1}{\sqrt{(A-2)!}} \det | u_{1} \ldots u_{\lambda-1} u_{\lambda+1} \ldots u_{\mu-1} u_{\mu+1} \ldots u_{A} |
$$

The matrix element $(u_{\lambda} u_{\mu} V(1-P) u_{\nu} u_{\rho})$ is again easily calculated by introducing the expansion (42) and coupling the two particles to a definite $J$. This gives

$$
\langle u_{\lambda} u_{\mu} V(1-P) u_{\nu} u_{\rho} \rangle = \sum_{pqrs} X_{p}^{\lambda} X_{q}^{\mu} X_{r}^{\nu} X_{s}^{\rho} \sum_{J}
$$

$$
C(i_{p} j_{q} J m_{\lambda} m_{\mu}) C(i_{r} j_{s} J m_{\nu} m_{\rho}) d_{m_{\lambda} + m_{\mu} - m_{\nu} + m_{\rho}}^{J}(\theta)
$$

$$
\langle p_{i_{p}} j_{q} V(1-P) r_{i_{r}} s_{j_{s}} \rangle
$$

(50)

This formula shows clearly that the labour of such a calculation increases very rapidly with the number of terms in the expansion (42). In the next section, we describe an approximate projected Hartree-Fock calculation for the light nuclei with $4 \leq A \leq 12$ for which it is possible to give some good arguments for choosing a special form for the orbitals such that the overlap matrix $O$ is very much reduced and the number of terms in the expansion (42) of the orbitals is small.

VI. PROJECTED HARTREE-FOCK CALCULATIONS FOR $4 \leq A \leq 12$

It has been said in the introduction that the main objective
of HF calculations in nuclei is the calculation of the shell-model potential and its eigenfunctions, starting from the nuclear Hamiltonian. In this way, the adjustable parameters are eliminated. However, one may also hope that HF calculations may solve in a satisfactory way the old problem of collective moments and transitions. It is well known that even in very light p-shell nuclei, electric quadrupole moments and transitions are often a factor two larger and faster, respectively, than the shell-model values. Several suggestions have been made how to improve the shell-model functions in order to reproduce the experimental collective quantities. The simplest of these suggestions is Nilsson's model in which the shell-model potential is allowed to deform. The deformation is treated as a new adjustable parameter and, in solving the problem of collective quantities, it sharpens the problem of the adjustable parameters. We know, however, that the HF potential has a definite size and a definite deformation which are calculated starting from the nuclear Hamiltonian. So we can calculate whether this deformation is the one needed to reproduce the collective quantities. In order to do so, it is necessary to calculate matrix elements of collective quantities with projected functions.

In this section we describe an approximate projected HF calculation for the nuclei $4 \leq A \leq 12$. These are the simplest nuclei to calculate and, on the other hand, they are already sufficiently heavy to show the problem of collective quantities in a clear way.

We start from the Hamiltonian for the internal energy

$$H = \sum_{i=1}^{A} T_i - T_{c.m.} + \frac{1}{2} \sum_{i \neq j}^{A} V_{ij}$$

where $T_{c.m.}$ is the kinetic energy of the centre of mass which is subtracted. As nucleon-nucleon interaction we choose an interaction of the Volkov type 17)

$$V_{12} = \left\{ -V_0 \exp \left[ \left( \frac{1}{a} \right)^2 \right] + V'_0 \exp \left[ -\left( \frac{1}{a'} \right)^2 \right] \right\} (1 - M + M P_x^2)$$

Volkov 17) has studied potentials of this type to be used in HF calculations for p-shell nuclei. The parameters $V_0$ and $V'_0$ are
chosen so as to fit approximately:

i) low-energy two-body scattering data;

ii) the binding energy and radius of $^4$He.

The exchange mixture contains only Wigner and Majorana components; $M$ is chosen so as to fit approximately the binding energy and radius of $^{16}$O.

We have used two sets of values for the parameters and label them Volkov and Brink, respectively. The last set was used by BRINK in some variational calculations with $\alpha$-particle type wave functions.  

<table>
<thead>
<tr>
<th></th>
<th>$V_0$</th>
<th>$a$</th>
<th>$V'_0$</th>
<th>$a'$</th>
<th>$M$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volkov</td>
<td>83.34</td>
<td>1.60</td>
<td>144.86</td>
<td>0.82</td>
<td>0.60</td>
</tr>
<tr>
<td>Brink</td>
<td>60</td>
<td>1.80</td>
<td>60</td>
<td>1.01</td>
<td>0.65</td>
</tr>
</tbody>
</table>

This interaction is purely central and independent of spin and isospin coordinates. The eigenfunctions of the Hamiltonian (51) can immediately be classified by WIGNER's supermultiplet theory. The lowest energy eigenfunctions belong to the most symmetric partition $[^f]$ and are eigenfunctions of both orbital ($L$) and spin ($S$) angular momentum separately, as well as of the total isospin $T$. How can the use of such a Hamiltonian in nuclear HF calculations be justified? In particular, can a HF calculation with a purely central Hamiltonian have any physical value?

There are some arguments why spin orbit forces can probably be neglected for the nuclei $4 \leq A \leq 12$, at least in first approximation. From intermediate coupling shell-model calculations it is well known that the partition quantum number $[^f]$ is very good for nuclei with $4 \leq A \leq 9$ and for the heavier p-shell nuclei it is still a fairly good quantum number. The lowest partition $[^f]$ contains the following $L$-values:
With the exception of $A = 9,10,11$, all the other nuclei correspond to partitions whose $L$-values increase by steps of two. This means that a spin-orbit force has no off-diagonal matrix elements, mixing different $L$-values. As a result, if $[f]$ is a good quantum number, $L$ is also a good quantum number for $A = 5,6,7,8,12$. Spin orbit forces then only play a role in lifting the degeneracy in $J$, without changing the wave functions, and can be neglected in a calculation of the wave functions. For the nuclei $A = 9,10,11$, the $L$-mixing due to the spin orbit force can easily be taken into account afterwards by perturbation theory. It is to be expected, however, that the results are less good for the heavier nuclei, since $[f]$ is becoming a less good quantum number.

Another possible justification for the neglect of the non-central forces follows from the HF calculations of Bassichis et al.\textsuperscript{6} described in Sec. 4. There we have seen that the HF orbitals for $^{8}\text{Be}$ obtained in a calculation with the realistic Tabakin force are almost exactly identical to those obtained in a calculation with a central Volkov force, and this is still approximately so in $^{12}\text{C}$. The non-central forces are thus of very little effect in determining the HF orbitals in light nuclei. We neglect them because this simplifies the calculation considerably.

Faessler\textsuperscript{21} has made HF calculations for $^{8}\text{Be}$ and $^{12}\text{C}$ starting from Volkov's interaction in a truncated Hilbert space ($0s$, $0p$, $1s$ $0d$, $1p$ $0f$). As a result he finds the following Slater determinant:
for $^8\text{Be}$ : $\phi = \text{det} \left| \psi_0^4 \varphi_0^4 \right|$ 

for $^{12}\text{C}$ : $\phi = \text{det} \left| \psi_0^4 \varphi_1^4 \varphi_{-1}^4 \right|$ \hfill (53)

with

$$
\begin{align*}
\psi_0 &= |os0\rangle + \alpha |ls0\rangle + \beta |odo\rangle \\
\varphi_0 &= |op0\rangle + \gamma |lp0\rangle + \delta |so0\rangle \\
\varphi_{\pm 1} &= |op_{\pm 1}\rangle + \varepsilon |lp_{\pm 1}\rangle + \zeta |of_{\pm 1}\rangle 
\end{align*}
$$

\hfill (54)

where $\alpha, \beta, \gamma, \varepsilon, \zeta$ are some numerical coefficients. The expansion of the orbitals contains only three terms. On the other hand, one easily sees that $S^2 \Phi = 0$, so that $J = L$. Taking an $L$-projection $P_L \Phi$, one has to calculate the overlap matrix $O_{\lambda \mu} = \langle u_\lambda | e^{-i \theta_j} | u_\mu \rangle$ which turns out to be very much reduced because of parity, spin and isospin selection rules. Thus both conditions for carrying out the angular momentum projection without much labour are fulfilled.

Instead of proceeding in two steps as described in the previous sections,

i) solve the HF equations, resulting in finding $\phi$,

ii) calculate with projected function $P_J \phi$

one can try to do both operations at once. This then means that one asks for the best function of the form $P_J \phi$ (where $\phi$ is a Slater determinant) in the sense that

$$
\delta \frac{\langle P_J \phi | H | P_J \phi \rangle}{\langle P_J \phi | P_J \phi \rangle} = 0
$$

\hfill (55)

This method will be called the projected Hartree-Fock (PHF) method (the projection being carried out before the Slater determinant $\phi$ is obtained). The previously described method will now be called the HFP
method (the projection being carried out after the HF determinant is obtained). The condition (55) leads to a very complicated set of equations for the HF orbitals $\psi_\lambda$, and there is no hope of solving these. In Sec. 3, it was shown how the complicated HF equations can be simplified in order to find the solution of a standard HF problem. Since the equations corresponding to the PHF problem are more difficult, one must obviously also resort to some simplifying approximations.

An approximation procedure for a PHF calculation with the Hamiltonian (51) for the nuclei $4 \leq A \leq 12$ is suggested in the following way. If we should use this Hamiltonian in a standard shell-model calculation, we would just get the ELLIOTT SU$_3$-functions as shell-model wave functions. This follows from the fact that both $\ell$ and $L$ are exact quantum numbers and there is only one function with a definite $L$ in the lowest partition (except for mass 10 for which some $L$-values occur twice. Now Elliott has shown that the SU$_3$-functions can be written as an $L$-projection from an intrinsic function $\Phi^0$. In all nuclei with $4 \leq A \leq 12$ it turns out that it is always possible to choose a single Slater determinant for the intrinsic functions. For the consecutive mass numbers, one has

\begin{align*}
A = 5 & \quad \phi^0 = \text{det} | (os)^4 (op)^n | \\
A = 6 & \quad \phi^0 = \text{det} | (os)^4 (op)^{n+} (op)^{p+} | \\
A = 7 & \quad \phi^0 = \text{det} | (os)^4 (op)^{n+} (op)^{p+} (op)^{n-} | \\
A = 8 & \quad \phi^0 = \text{det} | (os)^4 (op)^4 | \\
A = 9 & \quad \phi^0 = \text{det} | (os)^4 (op)^4 (opl)^n | \\
A = 10 & \quad \phi^0_{K=0} = \text{det} | (os)^4 (op)^4 (op)^{n+} (op-1)^{p+} |
\end{align*}

\begin{align*}
A = 10 & \quad \phi^0_{K=2} = \text{det} | (os)^4 (op)^4 (op)^{n+} (op)^{p+} |
\end{align*}
\( A = 11 \) \( \phi^0 = \det \begin{vmatrix} (sO)^4 \ (oPl)^4 \ (oP-l)^n^+ \ (oP-l)^n^- \end{vmatrix} \)

\( A = 12 \) \( \phi^0 = \det \begin{vmatrix} (sO)^4 \ (oPl)^4 \ (oP-l)^4 \end{vmatrix} \) (56)

In the case \( A = 10 \), there are two intrinsic states, respectively, with \( K = 0 \) and \( K = 2 \). It is immediately clear that the \( \phi^0 \) functions belong to the most symmetric partition, except for the \( K = 0 \) intrinsic state of \( A = 10 \). In fact, an intrinsic state belonging to the partition \([442]\) would be

\[ \det \begin{vmatrix} (sO)^4 \ (oP-l)^n^+ \ (oP-l)^n^- \end{vmatrix} + \det \begin{vmatrix} (sO)^4 \ (oP-l)^4 \end{vmatrix} \]

One can, however, easily show that both determinants give the same contribution when an even \( L \)-value is projected out and an opposite contribution if an odd \( L \)-value is projected out. This shows that one can take just one of these determinants as intrinsic states.

Now, at the beginning of this section, we have pointed out that the main objective of HF calculations was to eliminate the adjustable parameters, like, e.g., the size of the orbitals. If we should now take as trial functions just the shell-model function

\( \psi^0 = \Phi_L \phi^0 \) (57)

with \( \phi^0 \) given by (56) and treat the oscillator parameter as a variational parameter to be determined such that

\[ E^0(L) = \frac{\langle \psi^0_L | H | \psi^0_L \rangle}{\langle \psi^0_L | \psi^0_L \rangle} \] (58)

becomes minimum, we would have eliminated the adjustable size parameter. The procedure could be looked upon as an approximation to the PHF problem.

In the same way, we could consider different values for the oscillator parameters along the \( z \)-axis (symmetry axis \( \hat{z} \)) and along the \( x \)- and \( y \)-axes (symmetry plane \( \hat{y} \)). This means that one would use as trial function
where $\phi$ is given by (55) in which the following replacements are made:

\[ \text{oso} \rightarrow x_{000}(b_L, b_{\mu}) \]
\[ \text{opo} \rightarrow x_{001}(b'_L, b'_{\mu}) \]
\[ \text{opo} \pm 1 \rightarrow x_{l,\pm 1,0}(b''_L, b''_{\mu}) \]  \hspace{1cm} (60)

where $x_{n_{\mu}}, \wedge, n_2 (b_H, b_L)$ are eigenfunctions of the axially symmetric deformed harmonic oscillator potential. In this way, the deformation of the orbitals would be calculated. This would obviously be a better approximation to the PHP problem.

Variational calculations of this type, but without angular momentum projection have been carried out by VOLKOV\textsuperscript{17}. His calculations can be looked upon as an approximation to a standard HF calculation. Volkov found it very difficult to carry out the angular momentum projection. The reason is quite clear, since the orbitals (60) contain an infinite number of terms in their expansion in eigenfunctions of $l^2$. If, however, we truncate this expansion after a few terms, e.g.,

\[ x_{000}(b_L, b_{\mu}) = |\text{oso} > + \alpha |l\text{s}0 > + \beta |0\text{o}0 > + \cdots \]
\[ x_{001}(b'_L, b'_{\mu}) = |0\text{p}0 > + \gamma |l\text{p}0 > + \delta |0\text{f}0 > + \cdots \]
\[ x_{l,\pm 1,0}(b''_L, b''_{\mu}) = |0\text{p}1 > + \epsilon |l\text{p}1 > + \zeta |0\text{f}1 > + \cdots \]  \hspace{1cm} (61)

we know that the angular momentum projection is quite easy. Now, if $b_L$ and $b_H$ are both not very different from the length parameter $\ell$ in the spherical oscillator functions $|n_l m >$, the expansion will
have converged and the truncation will not change the physical meaning of the orbitals. Moreover, we see that the orbitals which we obtain in this way have exactly the same structure as those in (54) obtained in a standard HF calculation with the same interaction for Be and C. So we may be confident that our approximation procedure to the PHP problem is fairly accurate.

To summarize, we calculate the following energy:

\[ E_L(\alpha, \beta, \gamma, \delta, \epsilon, \zeta; k) = \frac{\langle P_L \phi | H | P_L \phi \rangle}{\langle P_L \phi | P_L \phi \rangle} \]  

(62)

where \( \phi \) is given by the Slater determinants in (56) in which the one-particle functions (Os0), (Op0), (Op±1) are replaced by the truncated expansions (61) of the deformed oscillator functions \( \chi_{000}, \chi_{001}, \chi_{1,\pm1,0} \). The parameters \( \alpha, \beta, \gamma, \delta, \epsilon, \zeta \) are treated as variational parameters, to be determined by the minimum condition for the energy \( E_L \).

It is to be remarked that the energy \( E_L^0(k) \) is obtained from \( E_L(\alpha, \beta, \gamma, \delta, \epsilon, \zeta, k) \) by putting all parameters \( \alpha = \beta = \gamma = \delta = \epsilon = \zeta = 0 \). The trial function \( \psi_L \) contains the shell-model function as a special case. Values for the parameters \( \alpha, \beta, \gamma, \delta, \epsilon, \zeta \) different from zero mean admixtures of higher configurations in the shell-model wave function.

VII. RESULTS OF PHP CALCULATIONS FOR NUCLEI WITH 4 \( \leq \) A \( \leq \) 12

1. Energies for the ground states

In Fig.1 are plotted the binding energies obtained for the ground states of the nuclei 4 \( \leq \) A \( \leq \) 12, and compared with the experimental binding energies which were corrected for Coulomb energies. The general behaviour of the calculated energies agrees quite well with the experimental binding energies, there being a cusp in the energy curve at A = 8. The details, however, show some discrepancies, the main one being a large dip both at A = 5,6 and at A = 9. In fact, both A = 6 and A = 9 would not be bound in contradiction with the experimental situation. A similar result was found by VOLKOV 17 and by BASSICHIS et al. 6 in their HF calculations,
FIGURE 1

Experimental

$E_L \ (\text{Volkov force})$
as we have discussed in Sec. IV. The explanation given there is also valid for this calculation.

In this calculation, all nuclei with $A \leq 10$ are prolate whereas $A = 11$ and $12$ are oblate. This is not a result of our calculation but was in fact assumed when writing down the determinants $\phi^o$ in (56). In general, it is possible to take another expression for $\phi^o$ (the "lowest weight" state of the SU$_3$-classification instead of the "highest weight" state). In (56) we have chosen that one which turned out to be a single Slater determinant. For some nuclei, $A = 6$ and $A = 10$, it is possible to write also an oblate Slater determinant from which the LS-coupling shell-model can be projected out. These are

\[
A = 6 \quad \phi' = \det |(os)^4 (opl)^n (op-l)^p| \\
A = 10 \quad \phi' = \det |(os)^4 (opl)^3 (op-l)^3| \tag{63}
\]

and $P_L \phi^o = P_L \phi'$ up to a multiplying constant. If the replacement (61) is carried through and (62) is minimized one finds that for both $A = 6$ and $A = 10$, the prolate minimum is lower by one or two MeV, respectively. This is in contrast with Volkov's results (without projection) who found the oblate solution to be lower for $9 \leq A \leq 12$. This is, anyway, not an important problem because both the oblate and prolate solutions have a very large overlap when a sharp $L$ is projected out.

In Table I we compare the energies for $4 \leq A \leq 8$ obtained from different variational methods:

1. **SM**: shell-model approximation (53);
2. **HF**: approximate Hartree-Fock. Trial function $\phi$ given by (56) in which the replacement (61) is made and $\alpha \beta \gamma \delta \epsilon \xi \eta \zeta \iota \kappa \lambda \mu \nu \xi \theta \upsilon \phi \chi \psi \omega$ are treated as variational parameters;
3. **HFP**: L-projection from HF.
4. **PHP**: approximate PHP (62).

-41-
Table I. Energies of ground states

<table>
<thead>
<tr>
<th>A</th>
<th>Sn</th>
<th>HFP</th>
<th>PHF</th>
<th>∆E</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>-27.9</td>
<td>-27.9</td>
<td>-28.0</td>
<td>0.1</td>
</tr>
<tr>
<td>5</td>
<td>-18.4</td>
<td>-20.7</td>
<td>-21.4</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>-19.3</td>
<td>-21.3</td>
<td>-25.3</td>
<td>6</td>
</tr>
<tr>
<td>7</td>
<td>-25.5</td>
<td>-33.1</td>
<td>-34.5</td>
<td>9</td>
</tr>
<tr>
<td>8</td>
<td>-39.6</td>
<td>-52.6</td>
<td>-54.3</td>
<td>14.7</td>
</tr>
</tbody>
</table>

In the last column $\Delta E = E_L^0 - E_L$ is the energy gained by introducing the parameters $\alpha, \beta, \gamma, \delta, \zeta$ in the shell-model function. The very large values show the importance of the admixtures of higher configurations in the shell-model function. The energy $\Delta E$ can also be called "deformation energy", it being the energy gain due to the deformation of the orbitals.

The energy gain (HFP-PHF) is quite small. We will see further that the deformation of the ground state in the PHF method is somewhat larger than in the HFP method and this larger deformation brings about a better agreement for the collective quantities.

2. Excited states (Volkov force)

Since the Hamiltonian is purely central, one obviously cannot expect a detailed agreement with the energies of excited states. Table II gives the calculated excitation energies, compared with some experimental "mean values", i.e., the mean for different $J$-values. It is interesting to see how well the energies $E_L$ satisfy the rotational band relation. In the pure shell-model, RACAH has shown that a central force leads to a pure $L(L+1)$ spectrum in the p-shell

$$E^0_L = E^0_0 + BL(L+1)$$

In Fig. 2 we have plotted both $E^0_L$ and $E_L$ as a function of $L(L+1)$ for $A = 9$ and $A = 11$. For $E_L$ one finds a considerable distortion of the rotational band, the state with $L = 3$ lying about 2 MeV too high.

Another interesting problem which can be treated by the PHF
method is the occurrence of non-normal parity states in the low-energy spectrum. In $^9$Be, there is a $\frac{1}{2}^+$ level at 1.7 MeV and a $\frac{5}{2}^+$ level at 3.03 MeV. Using the procedure described in the previous section, these levels would be described on the LS-coupling shell-model by the functions

$$P_L \det \begin{pmatrix} (\text{so})^4 & (\text{op})^4 & (150 - \sqrt{2} \text{odo}) \end{pmatrix}$$

with $L = 0$ and 2. Using the replacement (61), it would be natural to replace the last orbital $(\text{iso}) - \sqrt{2} (\text{odo})$ by the truncated expansion of $\chi_{002 \ell} (k_{\ell \ell}^m, k_{\ell m}^{\ell'}).$ Because of computer limitations this has not been done. The following energies are found:

<table>
<thead>
<tr>
<th>$L\pi$</th>
<th>$E_L^0$</th>
<th>$E_L$</th>
<th>$E_L^0 - E_L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-</td>
<td>-38.9</td>
<td>-49.7</td>
<td>10.8</td>
</tr>
<tr>
<td>2-</td>
<td>-37.5</td>
<td>-47.7</td>
<td>10.2</td>
</tr>
<tr>
<td>3-</td>
<td>-35.4</td>
<td>-42.6</td>
<td>7.2</td>
</tr>
<tr>
<td>4-</td>
<td>-32.5</td>
<td>-39.6</td>
<td>7.1</td>
</tr>
<tr>
<td>0+</td>
<td>-28.9</td>
<td>-45.4</td>
<td>16.5</td>
</tr>
<tr>
<td>2+</td>
<td>-28.8</td>
<td>-43.0</td>
<td>14.2</td>
</tr>
</tbody>
</table>
where we have also repeated the energies of the negative parity band. One sees that the even parity states lie well above the odd parity states in the shell-model approximation ($E^0_L$) but drop down low between the odd parity states when the states are allowed to deform. A very large gain in energy (16.5 MeV) is found for the $0^+$ level, although the outer orbital was not allowed to adjust its deformation to that of the other orbitals. An extra gain may be expected if the outer orbital is allowed to deform so that the experimental value of 1.7 MeV is quite well attainable.

3. Wave functions, size and deformation

The parameters $\alpha$, $\gamma$ and $\xi$ will be called size parameters since they admix an oscillator function with the same angular part to the lowest oscillator functions $\phi_0$ and $\phi_p$. In first order this amounts to only a change in the length parameter of the $\phi_0$ and $\phi_p$ oscillator functions. From $k$, $\alpha \gamma$ and $\xi$ one can thus calculate an effective length parameter for the inner ($\phi_0$) and outer ($\phi_p$, $\phi_{11}$) orbitals. Qualitatively, the same result is found for the behaviour of these effective length parameters, as was found by VOLKOV 17); the size of the inner orbitals increases with $A$, the size of the outer orbitals decreases with $A$. At $A = 12$, inner and outer orbitals have about the same length parameters.

The parameters $\beta$, $\delta$, $\zeta$, on the other hand, admix oscillator functions having a different angular part. These parts can be admixed by the quadrupole deformation of the potential. Thus $\beta$, $\delta$ and $\zeta$ can be called deformation parameters. The values of $\beta$ and $\delta$ for the ground states are given in Fig. 3 for the prolate solutions $5 \leq A \leq 10$. The deformation becomes maximum at $A = 8$. One sees that $\beta$ changes very much over the shell, whereas $\delta$ remains almost constant. Surprising also is that $\beta > \delta$. For a given prolate deformation, i.e., one definite $l_1 \neq l_{11}$, one finds that the expansion coefficients of $V_{000}$ and $\lambda_{11}$ satisfy $\beta < \delta$. So $\beta > \delta$ means that the HF potential is more deformed for the inner orbital ($\phi_0$) than for the outer orbital ($\phi_p$). It also means that there are more admixtures of configurations in which the $^4$He-core is excited. To have an idea of how much these admixtures take up of the total wave function, I give the decomposition of the ground state of $^7$Li:

-45-
65.7%  lowest configuration \((os)^4 (op)^3\)
24% configurations in which only s-particles are excited
6.8% configurations in which only p-particles are excited
3.5% configurations in which both s- and p-particles are excited

This large deformation of the inner orbitals seems surprising in view of the great stability of the K-particle. One can, however, understand this qualitatively as one expects a maximum interaction when the inner and outer orbitals have a probability distribution in space which overlap very well or, consequently, when the probability distributions for the orbital \(\chi_{000}\) and \(\chi_{001}\) have similar deformation. Now, the orbital \(\chi_{000}(k_2, \ell_{11})\) is spherical if
whereas $X_{601}(\ell_\perp, \ell_{\|})$ is deformed when $\ell_\perp = \ell_{\|}$. So if $X_{600}(\ell_\perp, \ell_{\|})$ wants to have the same deformation as $X_{601}(\ell_\perp, \ell_{\|})$, one must take $\ell_\perp = \ell_{\|}$. Now if $\ell_\perp \neq \ell_{\|}$, the $X_{600}$ orbital is even more deformed and one needs a larger $|\ell_\perp - \ell_{\|}|$ difference for $X_{600}$ to obtain the same deformation of the mass distribution.

Tables with the values of the parameters $\chi, \rho, \gamma, \bar{c}, \zeta$ and $l_r$ are given in Ref. 24 for $4 \leq A \leq 8$ and in Ref. 25 for $A = 12$. They are not reproduced here because they are quite long.

To conclude this section, we remark that as a result of these PHF calculations one invariably finds $\beta$ and $\delta$ larger for the ground state than for the excited states. In fact $\beta$ and $\delta$ decrease monotonically as $L$ increases within a "rotational band". This is exactly the opposite of what one expects for a rotational band from the centrifugal force. This result is probably an indication of the fact that the states $\ell \phi$ are not very real, rotational states.

VIII. COLLECTIVE MOMENTS AND TRANSITIONS. FORM FACTORS FOR HIGH-ENERGY ELECTRON SCATTERING.

The PHF functions obtained in the way described above have a strongly deformed intrinsic state and one may ask whether the electromagnetic collective E2 moments and transitions can be explained. If so, this would mean that the problem of the collective quantities in the shell model has its origin in the fact that the shell-model potential was not calculated but chosen incorrectly. That this is indeed so will be seen by calculating several collective quantities in $^6$Li, $^7$Li and $^{12}$C. Similar calculations are presently being carried out for $^9$Be and preliminary results show good agreement for this nucleus also.

Before considering collective quantities, one may, however, wonder whether the large admixtures of higher configurations have not disturbed the agreement which existed between the shell-model predictions and experimental magnetic dipole moments and transitions. That this is not so can be seen as follows. The magnetic dipole operator

$$\mu = \sum_p \ell_z p + \mu_p \sum_p \sigma_z p + \mu_n \sum_n \sigma_z n$$
consists of an orbital and a spin part. The spin part can be rewritten as follows:

$$\mu_{\text{spin part}} = \frac{\mu_p + \mu_n}{2} \sum_i \sigma_z + \frac{\mu_p - \mu_n}{2} \sum_i \sigma_z \tau_3$$

where the sums run now over all nucleons. The new operators $\sum \sigma_z$ and $\sum \sigma_z \tau_3$ are, however, infinitesimal operators of the group $SU_4$. The matrix elements of these operators are consequently completely determined by the transformation properties of the PHF functions under the group $SU_4$ and not by the detailed structure of the functions (in the same way that the matrix elements of $L_z$, e.g., between functions which have definite transformation properties under rotations are determined by these transformation properties). This means that the spin part of the magnetic moment operator is exactly the same for the PHF as for the shell-model LS-coupling functions. The orbital part, on the other hand, is usually much smaller and has no matrix elements between different shell-model configurations. This means that the change is only of second order in the variational parameters. The total change is quite small (the above argument is obviously also applicable to allowed $\mathcal{M}$-transitions, the operators $\sum \tau$ and $\sum \sigma \tau$ being infinitesimal operators of $SU_4$).

Detailed calculations of collective moments and transitions, as well as form factors for elastic and inelastic electron scattering have been described in the literature \(^{26},^{27}\). They will not be copied here. The agreement between calculated and experimental data is quite satisfactory, making a considerable improvement as compared with the shell-model functions. This shows that admixtures of higher configurations are also important for low-lying states. Standard shell-model calculations cannot take these into account because of computational limitations. They are, however, easily incorporated through a HF calculation.
REFERENCES


5) M. BOUTEN and P. VAN LEUVEN, Physica 34, 461 (1967).


23) G. RACAH, L. Farkas memorial volume (Research Council, Israel 1951).


