Shapes and Symmetries of Light Nuclei*

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We demonstrate that the existence of symmetries under the operations T, $P\exp(-i\pi J_y)$, and $\exp(i\pi J_z)$ in the Hartree-Fock densities of even-even $N=Z$ nuclei follows directly from two indisputable features of any effective shell-model interaction, viz., the general exchange nature and the short range. We show that this implies that one should not expect parity mixing in Hartree-Fock ground state wave functions for these nuclei. Finally, we demonstrate that these same features of the interaction allow us to predict the shapes of the Hartree-Fock densities.

INTRODUCTION

OVER the past several years there has been considerable progress in our understanding of the structure of light nuclei through studies employing the Hartree-Fock (HF) approximation.[1] In these calculations special emphasis has been placed on the even-even, $N=Z$ nuclei ($4n$ nuclei) which exhibit a large gap in the single-particle HF energies between occupied and unoccupied orbitals. Such a large gap is not observed for other types of nuclei and, in fact, self-consistent Hartree-Fock-Bogoliubov (HFB) calculations[2] converge to HF solutions (i.e., no-pairing solutions) only for the $4n$ nuclei. In the s-d shell, these HF solutions exhibit a very interesting alternation of shape; Ne^{20}, Si^{28}, and Ar^{36} have spheroidal (axially-symmetric) density distributions, while Mg^{24} and S^{32} have ellipsoidal (triaxial) density distributions.

In all of the HF calculations to date, certain symmetries have always been assumed. The single-particle densities have been taken to be invariant under:

(1) time-reversal; T,

(2) reflection through a plane, e.g., the x-z plane; $P\exp(-i\pi J_y)$, and

(3) rotation by π about an axis in the plane of reflection symmetry, e.g., the z axis; $\exp(i\pi J_z)$,

where P in (2) is the parity operator. Symmetries (2) and (3) above together imply that the y-z plane is also a plane of reflection symmetry. The major experimental evidence leading to the assumption of these symmetries is the lack of any low-lying 1^+ states in the spectra of the $4n$ nuclei. The immense increase in labor involved in dropping the assumption has inhibited the use of more general trial functions to test its validity.

Inasmuch as the effective shell-model Hamiltonian H is invariant under all of these symmetry operations, it might appear that there have been no assumptions involved by taking the HF density to be invariant under the same symmetry operations. This clearly is not the case. For any odd-A nucleus the spin of the last nucleon precludes time-reversal invariance of the density. In all HF treatments of rotational nuclei, we seek a description of a deformed intrinsic state from which a rotational band can be projected, a procedure which obviously relaxes the requirements of rotational invariance for the HF density. There have also been several suggestions to the effect that an improved HF density may be obtained by allowing parity mixing in the single-particle orbitals and then projecting states of both parities from the same intrinsic wave function.[3] In this paper we address ourselves to the problem of determining which of the symmetry operations which commute with H also commute with the HF density ρ, a problem which can only be treated by studying the dynamical features of H.

We shall demonstrate that the three symmetries listed above follow from two simple and well-known properties of all effective shell-model interactions; the exchange nature and the finite range. From this other interesting results follow, such as the alternation of shapes described above and the lack of parity mixing in nuclear HF wave functions.

SINGLE-PARTICLE ORBITALS AND SYMMETRIES

Since the HF wave function $|\Phi\rangle$ is arrived at by minimizing $\langle\Phi|H|\Phi\rangle$, $|\Phi\rangle$ will adjust itself to take maximum advantage of the most attractive features of the effective interaction V. Since the dominant part of the effective interaction is the central interaction V_c we should first investigate the constraints imposed on $|\Phi\rangle$ by the requirement that the attraction due to V_c is maximized, and then maximize the attraction due to the noncentral parts of V subject to these constraints.

First, let us consider the case of a purely central force and study the effect on $|\Phi\rangle$ of the exchange nature of V_c. For all exchange mixtures in use, V is much more attractive in even relative space states than it is in odd relative space states and, in fact, it is usually repulsive in the latter. Two nucleons in the same space orbital can only interact through even relative space states,

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[1] For an excellent summary of HF calculations in light nuclei, see G. Ripka, *Advances in Nuclear Physics* (Plenum Press, Inc., New York, 1968), Vol. 1, and references therein.

[2] L. Satpathy, D. Goss, and M. K. Banerjee, Phys. Rev. (to be published).

[3] K. Bleuler, in *Proceedings of the International School of Physics "Enrico Fermi," Course 36* (Academic Press Inc., New York, 1966).

TABLE I. Cartesian orbitals in the $2s$-$1d$ shell used as examples in the text. The normalization constant $N=2^{-1/2}b^{-3/2}\pi^{-3/4}$.

Type (a) 2 quanta in one direction	Type (b) 1 quantum in each of two directions
$(r \mid 200)=N[(2x^2/b^2)-1]\exp(-r^2/2b^2)$	$(r \mid 011)=2N(yz/b^2)\exp(-r^2/2b^2)$
$(r \mid 020)=N[(2y^2/b^2)-1]\exp(-r^2/2b^2)$	$(r \mid 101)=2N(zx/b^2)\exp(-r^2/2b^2)$
$(r \mid 002)=N[(2z^2/b^2)-1]\exp(-r^2/2b^2)$	$(r \mid 110)=2N(xy/b^2)\exp(-r^2/2b^2)$

while two nucleons in different space orbitals interact through odd relative states 10/16 of the time and through even relative states only 6/16 of the time. From this it follows that a given orbital will be fully occupied (i.e., occupied by neutrons and protons of both spins) in $|\Phi\rangle$, leading to a $[4,4,4,\cdots]$ $SU(4)$ symmetry. Bar-Touv and Levinson[4] have shown by this argument that the exchange nature of the force accounts for the observed gap between the energies of the occupied and unoccupied orbitals in HF solutions for the $4n$ nuclei in the s-d shell. For our purposes, the important result is that the HF wave function $|\Phi\rangle$ is scalar in spin and isospin for $4n$ nuclei, consequently the symmetries of $|\Phi\rangle$ are determined by the space wave functions of the single particle orbitals.

To examine the functional form of the space orbitals, we may proceed as follows. We consider the space orbitals to be constructed from a complete set of states in a representation where l and m are good quantum numbers. We then consider the dominant attractive matrix elements of V_c and adjust the coefficients in the expansions of the orbitals to maximize these matrix elements. This approach is described in detail in the appendix. Here we present a more qualitative argument, using s-d shell wave functions as examples, which produces the same results.

The dominant feature of the space dependence of V_c is its short range. Considering the discussion of the effect of exchange, we first maximize the expectation value of V_c between two particles in the same orbital. Because of the short range, the wave function is maximized when the density distribution is as compact as possible. This, then, is the primary constraint on the space wave functions; they must have the minimum spatial extent consistent with the requirements of the exclusion principle.

The space wave functions in the s-d shell can be expressed in terms of a basis set of Cartesian wave functions; for convenience we use oscillator wave functions. These are of two types; three of type (a) corresponding to two quanta in some one direction and three of type (b) corresponding to one quantum in each of two directions. The basis functions are displayed in Table I. Figure 1 shows schematically the density distributions for typical orbitals of each type. It is clear that the density of a type-(a) orbital is more compact than that of a type-(b) orbital. Figure 2 shows schematically the density distributions for a linear combination of the Cartesian basis functions, in this case chosen to be an eigenfunction of angular momentum. It is clear that these densities are much less compact. In fact any linear combination of two or more of the Cartesian basis functions, which is not equivalent to a rotated Cartesian basis function, leads to a less compact density than that which we obtain with single Cartesian functions. From this it follows that the Cartesian wave

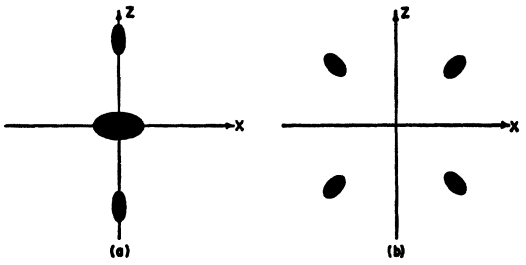

FIG. 1. Schematic representations of the density distributions arising from the Cartesian orbitals of type (a) and (b) discussed in the text and displayed in Table I. The examples shown correspond to (a) two quanta in the z direction and (b) one quantum each in the x and z directions.

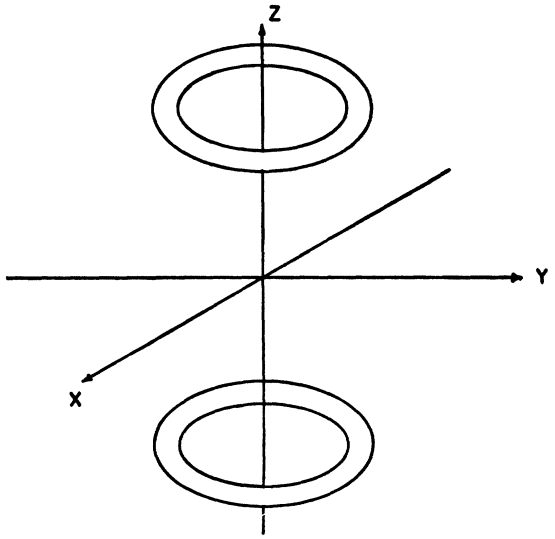

FIG. 2. A schematic representation of the effect of taking a linear combination of two orbitals of type (b) to form an orbital with sharp angular momentum, in this case the density corresponds to either the $1d_1$ or the $1d_{-1}$ orbital. A three-dimensional sketch is employed to illustrate the smearing of the density due to the cylindrical symmetry about the z-axis.

[4] J. Bar-Touv and C. A. Levinson, Phys. Rev. 153, 1099 (1967).

functions are the correct space wave functions for the HF orbitals. Of course, linear combinations of the filled orbitals may always be used without changing $|\Phi\rangle$.

Each of the Cartesian orbitals in invariant under the symmetries T, $\exp(i\pi L_z)$, $\exp(-i\pi L_y)$, and P. Since each filled orbital is invariant under these operations, the entire determinental wave function $|\Phi\rangle$ is also invariant under these operations. Since the density is scalar in spin space, it is also invariant under $\exp(i\pi J_z)$ and $\exp(-i\pi J_y)$. These conclusions correspond to the first two conditions in the Appendix, namely, time-reversal invariance and the fact that, in the expansion of an orbital, only components with m's differing by 2 appear. To determine whether the density is invariant under $\exp(-i\pi L_y)$ $[\exp(-i\pi J_y)]$ or $P\exp(-i\pi L_y)$ $[P\exp(-i\pi J_y)]$, we must inquire as to the relative phase of components from different shells. Through a careful study of the types of components introduced by possible parity mixing, we show in the Appendix that these components must be relatively real. This result demonstrates that $P\exp(-i\pi L_y)$ $[P\exp(-i\pi J_y)]$ is the correct choice.

The inclusion of a spin-orbit force eliminates the symmetries involving the orbital angular momentum operator. However, since an $\mathbf{l}\cdot\mathbf{s}$ force commutes with the remaining symmetry operators, they survive. Consequently, we have demonstrated the necessity for the HF density to be invariant under the three symmetries under consideration, viz., T, $\exp(i\pi J_z)$ and $P\exp(-i\pi J_y)$.

PARITY MIXING IN THE HF ORBITALS

We now wish to investigate the conjecture that an improved HF description might be obtained by allowing the HF orbitals to be constructed with mixed parity.[3] The prime candidate to provide a field which could accomplish this is the tensor force. The field-producing term could, in principle, be of the form $\mathbf{r}\cdot\boldsymbol{\sigma}$ or $\mathbf{p}\cdot\boldsymbol{\sigma}$. In the latter case, the coefficients of components from shells of different parity will be relatively imaginary, a condition ruled out by the symmetries $P\exp(-i\pi J_y)$ and T. In the former case, the HF density must give up time-reversal symmetry. In either case, while parity mixing could increase the attraction due to the tensor force, it would decrease the attraction due to the central interaction. Because of the dominance of the central interaction, we would not expect to observe parity mixing in nuclear HF calculations for the ground band using any reasonable effective interaction. This expectation is borne out in the calculations of Bassichis, Kerman, and Svenne,[5] who find no advantage to parity mixing unless the tensor force is increased to nearly twice its normal strength.

[5] W. H. Bassichis, A. K. Kerman, and J. P. Svenne, in *Proceedings of the International Conference on Nuclear Physics, Gatlinburg, Tenn., 1966* (Academic Press Inc., New York, 1967), p. 855.

TABLE II. Relative strengths of the matrix elements $\langle n_x n_y n_z(1), m_x m_y m_z(2) \mid v \mid n_x' n_y' n_z'(1), m_x' m_y' m_z'(2)\rangle$ of simple two-body forces between Cartesian states. Each column is normalized to the $\langle 002, 002 \mid v \mid 002, 002\rangle$ matrix element; in a reasonable representation of the effective two-nucleon force, the strength of the δ-function interaction is much greater than the core polarization term in the last column. The R is this term is the radius where the p-shell density is a maximum.

	δ function	$\delta(r_1-R)\delta(r_2-R)\times\cos^2\theta_{12}$
$\langle 002, 002 \mid v \mid 002, 002\rangle$	1	1
$\langle 002, 011 \mid v \mid 002, 011\rangle$	0.341	1.015
$\langle 002, 110 \mid v \mid 002, 110\rangle$	0.146	0.702
$\langle 002, 020 \mid v \mid 002, 020\rangle$	0.220	0.797
$\langle 011, 011 \mid v \mid 011, 011\rangle$	0.878	1.386
$\langle 011, 101 \mid v \mid 011, 101\rangle$	0.293	1.101

SHAPES OF THE HF DENSITIES

The HF density may have additional symmetries compatible with the three studied here when certain combinations of orbitals are filled. One such possibility is the existence of an axis of rotational symmetry. Clearly, for any single Cartesian orbital, such an axis can always be found. For densities composed of more than one orbital, the interaction between orbitals must be studied to determine which orbitals are filled. As a guide, the matrix elements of a δ-function potential are presented in Table II.

At the beginning of the s-d shell, for Ne^{20}, only one orbital will be filled. From the arguments above, or from Table II, we see that this orbital will be of type (a) and, for convenience, we choose it to correspond to 2 quanta in the z direction. The resulting density has rotational symmetry about the z axis and a positive quadrupole moment; i.e., it is prolate and axially symmetric.

When we fill a second orbital to form Mg^{24}, we must include the interactions between the orbitals to determine the minimum energy. As can be seen from Table II, an ambiguity arises from the use of just the δ-function force. The same binding energy is obtained either by filling one orbital of type (a) and one of type (b) with one quantum in the same direction, or by filling two orbitals of type (a). The fact that the range of the actual force is not zero, however, increases the relative importance of the overlap between different orbitals and hence favors filling one orbital of type (a), say, $|002)$, and one of type (b), $|011)$. The resulting density no longer has any axis of rotational symmetry. It is interesting to note that core-polarization effects on the effective matrix elements of the type discussed by Kuo and Brown[6] leads to the same conclusions as the nonzero range; for comparison matrix elements of this correction are included in Table II.

[6] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **85**, 40 (1966).

TABLE III. Results of HF calculations (Ref. 2) for $N=Z$ even-even nuclei in the $2s$-$1d$ shell. The effective interaction is taken to have a Yukawa radial dependence with range 1.4 F, and an exchange mixture giving the following depths in different spin space states: V triplet even $=-43.0$ MeV, V singlet even $=-31.5$ MeV, V triplet odd $=17.8$ MeV, and V singlet odd $=37.4$ MeV. Oscillator wave functions are used with the length parameter b chosen to give the correct rms radius. For triaxial nuclei, the axes are chosen so that the magnitude of Q_0 is greater than that of Q_{22}.

Nucleus	Shape	Q_0 in units of b^2	Q_{22} in units of b^2
Ne^{20}	Prolate axial	7.8	0
Mg^{24}	Triaxial	8.8	5.4
Si^{28}	Oblate axial	−11.4	0
S^{32}	Triaxial[a]	∼0	∼0
Ar^{36}	Oblate axial	−6.4	0

[a] The vanishing of the quadrupole moments does not imply spherical symmetry as higher moments, especially the hexadecapole moments, are nonvanishing.

Repeated applications of the above arguments through the s-d shell lead to the following predictions for the shapes of the HF densities for $N=Z$ $4n$ nuclei: Si^{28} will be oblate with axial symmetry. S^{32} will not have axial symmetry, and Ar^{36} will be prolate with axial symmetry. The results of actual HF calculations are presented in Table III, and these results agree with those expected from our arguments.

An extension of these arguments to interactions between major shells leads one to expect the four-particle–four-hole intrinsic state of O^{16} to be composed of an oblate density for the eight p-shell particles and the four s-d shell particles occupying an orbital of type (a) which has its density in the plane of the p-shell density, leading to an over-all density which has no axis of rotational symmetry. This result is also borne out in explicit calculations.[7]

SUMMARY

Relying only on the main features of the effective shell-model interaction, features common to all potentials currently in use, we have shown that the HF densities of $4n$, $N=Z$ even-even nuclei will be invariant under the symmetry operations T, $\exp(i\pi J_z)$ and $P\exp(-i\pi J_y)$. The simple arguments presented in the body of the paper are not restricted in their validity to s-d shell nuclei nor especially to s-d shell harmonic-oscillator wave functions; these have been used as an illustrative example. The arguments presented in the appendix clearly are not restricted to any single major shell. We also have shown that parity mixing is not expected to give any advantage in these nuclei and that the qualitative behavior of the shapes of the HF densities in the s-d shell may also be understood from the dominant features of the effective interaction.

[7] G. J. Stephenson, Jr., and M. K. Banerjee, Phys. Letters **24B**, 209 (1967).

APPENDIX

The effect of the exchange nature of the effective interaction, as discussed in the text, is to lead to occupation of each space orbital four times, i.e., to $[4,4,4\cdots]$ $SU(4)$ symmetry for the HF wave function in the light $4n$ nuclei discussed in this paper. As a result, the density and the single-particle Hamiltonian h are scalar in spin-isospin space and we need only consider the space wave functions of the occupied orbitals and the symmetry operations T, $P\exp(-i\pi L_y)$, and $\exp(i\pi L_z)$.

Let us write the space wave function of an occupied orbital as

$$u_i(\mathbf{r})=\sum C_{nlm}{}^i\,|\,nlm\rangle, \tag{A1}$$

where the $|\,nlm\rangle$ form a complete set of suitably chosen functions and where we follow the Condon-Shortley phase conventions for the angular functions, i.e.,

$$\langle lm'\,|\,L\pm\,|\,lm\rangle\geq 0 \tag{A2}$$

and

$$T\,|\,nlm\rangle=(-)^m\,|\,nl-m\rangle.$$

The condition that the density and h are invariant under the symmetries in question leads to the requirement that the following three functions:

$$Tu_i(\mathbf{r})=\sum(-)^m C_{nlm}{}^{i*}\,|\,nl-m\rangle, \tag{A3}$$

$$P\exp(-i\pi L_y)u_i(\mathbf{r})=\sum(-)^m C_{nlm}{}^i\,|\,nl-m\rangle, \tag{A4}$$

and

$$\exp(i\pi L_z)u_i(\mathbf{r})=\sum(-)^m C_{nlm}{}^i\,|\,nlm\rangle, \tag{A5}$$

must either be multiples of $u_i(\mathbf{r})$ or else linear combinations of occupied orbitals at the same energy. In the latter event, suitable linear combinations of the occupied orbitals may be chosen to make the $u_i(\mathbf{r})$ eigenfunctions of the three symmetry operators. This is possible because, for space wave functions carrying integral angular momentum,

$$T^2u_i(\mathbf{r})=[P\exp(-iL_y)]^2u_i(\mathbf{r})=u_i(\mathbf{r}).$$

Requiring that the $u_i(\mathbf{r})$ be eigenfunctions of the symmetry operators, with eigenvalue $+1$, Eqs. (A3)–(A5) lead to the following relations on the expansion coefficients:

$$C_{nl-m}{}^i=(-)^m C_{nlm}{}^{i*}, \tag{A6}$$

$$C_{nlm}{}^i \text{ is real.} \tag{A7}$$

"The nonzero $C_{nlm}{}^i$'s have m's differing by multiples of 2, i.e., are all even or are all odd." (A8)

To show that the HF density is invariant under the three symmetries, we need to show that the relations (A6)–(A8) follow from the nature of the effective two-body interaction.

The expectation value of the energy is given by

$$\langle\phi \mid H \mid \phi\rangle=\sum_i\langle i \mid H_0 \mid i\rangle+\sum_i\langle ii \mid v \mid ii\rangle + \sum_{i>j}\langle ij \mid v \mid ij\rangle, \quad \text{(A9)}$$

where the sums are over occupied single-particle orbitals. The spin and isospin indices are suppressed. H_0 is the single-particle part of the shell-model Hamiltonian H, the second term is the interaction of nucleons in identical space orbitals through the effective interaction v, and the last term is the interaction between nucleons in different space orbitals. Since H_0 is invariant under the symmetry operations in question, its effect on the $C_{nlm}{}^i$ will not affect the symmetry properties of h. As described in the text, the main attraction will come from the second term in (A9), hence the symmetry properties of the orbitals will be determined by it; the third term will primarily affect the equilibrium shapes in nuclei with more than one orbital occupied.

The second term in (A9) involves a spin-isospin sum over space symmetric states which may be written as

$$\sum_i\langle ii \mid v \mid ii\rangle=6\sum_i A_i{}^*(l_1l_2;\,LM)\,A_i(l_3l_4;\,LM) \times\langle(l_1l_2)LM \mid v_+ \mid (l_3l_4)LM\rangle, \quad \text{(A10)}$$

where

$$A_i(l_1l_2;\,LM)=\sum C_{n_1l_1m_1}{}^iC_{n_2l_2m_2}{}^i\begin{bmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M\end{bmatrix}\sigma_{12} \quad \text{(A11)}$$

is the amplitude of the space-symmetric vector coupled state $\mid (l_1l_2)LM\rangle$ in $\mid ii\rangle$. The symbol

$$\begin{bmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M\end{bmatrix}$$

stands for the Clebsch-Gordan coefficient, and σ_{12} is a normalization factor to account for the possibility that 1 and 2 may be identical orbitals. The interaction potential v_+ is one-half of the sum of the singlet-even and triplet-even interaction potentials.

To maximize the attraction in (A10), we must maximize first the amplitude of the most attractive matrix element of v_+, then, consistent with this, maximize the amplitude of the next most attractive matrix element, and so on. There are certain features of the two-body matrix elements which are true for any form of effective shell-model interaction likely to be considered seriously, and it is upon these that we wish to draw:

(a) The biggest matrix elements are

$$\langle l^2L=0 \mid v_+ \mid l^2L=0\rangle,$$

those for zero-coupled angular momentum.

(b) The phase of the matrix element

$$\langle l^2L=0 \mid v_+ \mid l'^2L=0\rangle$$

is $(-)^{l-l'}$ times an attractive matrix element.

(c) Among the matrix elements in space symmetric states, $\langle(ll')L \mid v_+ \mid (ll')L\rangle$, the biggest are those for which $l+l'+L$ is even.

(d) Among the matrix elements of type (c), the biggest is that for which $L=\mid l-l'\mid$.

These features are basically the result of the fact that, beyond the separation distance which is small compared to the size of nuclei, the effective potential falls off smoothly and rapidly. The "core polarization correction"[6] arising in calculations where major shell mixing is not allowed does not change these features.

Since the $\langle l^2L=0 \mid v_+ \mid l^2L=0\rangle$ matrix elements are the most attractive, the variational procedure will automatically make the amplitudes

$$A_i(ll;\,00)=\sum_m(-)^{l-m}C_{nlm}{}^iC_{nl-m}{}^i(2l+1)^{-1/2} \quad \text{(A12)}$$

as large as possible. However, we are in no position to comment on the magnitudes of the $C_{nlm}{}^i$ without a knowledge of the detailed dependence of H_0 and the matrix elements of v_+ on n and l. In particular, we should keep

$$N_{nl}{}^i=\sum_m\mid C_{nlm}{}^i\mid^2, \quad \text{(A13)}$$

the weight of the state (n,l) in u_i, fixed in our attempt to maximize the magnitude of (A12). Multiplying (A13) by a Lagrange multiplier, adding to (A12) and differentiating with respect to $C_{nlm}{}^i$, we get the relation

$$C_{nl-m}{}^i=\mu_{nl}{}^i(-)^{l-m}C_{nlm}{}^{i*}. \quad \text{(A14)}$$

The unknown factor $\mu_{nl}{}^i$ may depend upon n and l, but not on m. By reflecting the sign of m in (A14), we see that $\mid\mu_{nl}{}^i\mid=1$. Substituting (A14) in (A12), we get

$$A_i(ll;\,00)=\sum_l(2l+1)^{-1/2}\mu_{nl}{}^iN_{nl}{}^i. \quad \text{(A15)}$$

The preceding considerations guarantee that the diagonal $L=0$ matrix elements contribute to the attraction as much as possible. Turning to the off-diagonal $L=0$ matrix elements, we find that in order to guarantee that the terms

$$A_i(ll;\,00)\,A_i{}^*(l',\,l';\,00)\,\langle l'^2L=0 \mid v_+ \mid l^2L=0\rangle$$

are all attractive we must have

$$\mu_{nl}{}^i=(-)^le^{i\alpha}, \quad \text{(A16)}$$

where the real phase factor α is independent of l and n. Combining (A16) with (A14), we find that we have derived the relation (A6), the condition that $u_i(\mathbf{r})$ be an eigenfunction of T, the time-reversal operator. This, in its turn, guarantees that the HF density is invariant under time reversal.

To derive the remaining two symmetries, viz., $P\exp(-i\pi L_y)$ and $\exp(i\pi L_z)$, we must consider the

$L\neq 0$ matrix elements. Let us first consider the amplitude for $L\neq 0$ and $M=0$:

$$A_i(ll';\,L,\,M=0)=\sum_m\left(C_{nlm}{}^iC_{n'l'-m}{}^i\begin{bmatrix} l & l' & L\\ m & -m & 0\end{bmatrix}+C_{nl-m}{}^iC_{n'l'+m}{}^i\begin{bmatrix} l & l' & L\\ -m & m & 0\end{bmatrix}\right). \quad \text{(A17)}$$

Using (A6) and the relation

$$\begin{bmatrix} l & l' & L\\ m & -m & 0\end{bmatrix}=(-)^{l+l'-L}\begin{bmatrix} l & l' & L\\ -m & m & 0\end{bmatrix}, \quad \text{(A18)}$$

we may rewrite

$$A_i(ll';\,L,\,M=0)=\sum_m(-)^m\begin{bmatrix} l & l' & L\\ m & -m & 0\end{bmatrix}\times\{C_{nlm}{}^iC_{n'l'm}{}^{i*}+(-)^{l+l'-L}C_{nlm}{}^{i*}C_{n'l'm}{}^i\}. \quad \text{(A19)}$$

Because of the property (c) of the matrix elements $\langle(ll')_+L\mid v\mid(ll')_+L\rangle$ the amplitude (A17) should have the maximum magnitude for $l+l'+L=$even. For a given value of $\mid C_{nlm}{}^iC_{n'l'm}{}^i\mid$, the expression in curly brackets in (A19) has the maximum magnitude when

$$C_{nlm}{}^iC_{n'l'm}{}^{i*}=\text{real} \quad \text{(A20)}$$

or, in other words,

$$C_{nlm}{}^i=\mid C_{nlm}{}^i\mid\exp[i\phi(m)], \quad \text{(A21)}$$

where the phase $\phi(m)$ is independent of n and l. Next we consider the amplitude for $L\neq 0$ and $M\neq 0$, which is

$$A_i(ll';\,L'M)=\sum_m\left(C_{nlm}{}^iC_{n'l'M-m}{}^i\begin{bmatrix} l & l' & L\\ m & M-m & M\end{bmatrix}+C_{nlM-m}{}^iC_{n'l'm}{}^i\begin{bmatrix} l & l' & L\\ M-m & m & M\end{bmatrix}\right). \quad \text{(A22)}$$

Ordinarily there is no simple phase relationship between the two Clebsch-Gordan coefficients, except in the case of $L=\mid l-l'\mid$, where

$$\begin{bmatrix} l & l' & L\\ m & M-m & M\end{bmatrix}=(-)^{l-m}\times(\text{positive number}). \quad \text{(A23)}$$

Using (A23) we may rewrite (A22) as

$$A_i(ll';\,L,\,M)=\sum_m\{C_{nlm}{}^iC_{n'l'M-m}{}^i(-)^{l-m}x+C_{nlm-m}{}^iC_{n'l'm}{}^i(-)^{l-m+M}y\}, \quad \text{(A24)}$$

where x and y are the magnitudes of

$$\begin{bmatrix} l & l' & L\\ m & M-m & M\end{bmatrix}\text{ and }\begin{bmatrix} l & l' & L\\ M-m & m & M\end{bmatrix}.$$

The property (d) implies that (A24) should be as large in magnitude as possible. To arrange this the two terms in the curly bracket in (A24) should have the same phase. Because of (A21) this means that M should always be even. To ensure this, we must have either only even m's or only odd m's in (A1), i.e., the condition (A8) must be fulfilled.

Finally if we want the summands in (A24) to have the same phase, the phase $\phi(m)$ must be of the linear form

$$\phi(m)=\phi_0+\phi_1 m. \quad \text{(A25)}$$

Such a phase can be eliminated by a rotation of the system about the Z axis through an angle $-\phi_1$ and multiplication of u_i with the factor $\exp(-i\phi_0)$. This means that it is possible to arrange that $C_{nlm}{}^i$ is real. Therefore, by considering only the phases of the coefficients $C_{nlm}{}^i$ in the expansion (A1) and seeing how the attraction among four particles in the same orbit can be maximized, we have demonstrated the need for the conditions (A6)–(A8) and, thereby, the need for the symmetries T, $P\exp(-i\pi J_y)$ and $\exp(i\pi J_z)$.