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# DEFORMATIONS IN PERTURBATION THEORY

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**Abstract:** The Nilsson model for light nuclei is studied from the point of view of perturbation theory. Core wave functions are calculated using realistic two-body interactions. It is found that the Nilsson model describes the core energy and quadrupole polarization quite well, but that the assumption of constant volume upon deformation is poor for calculating electric monopole amplitudes.

## 1. Introduction

Recently there has been considerable progress in the theoretical description of the wave function of light nuclei. A surprising fact to emerge is that the simple wave functions of Nilsson [1]) give an essentially correct picture. Both Hartree-Fock calculations, which find an intrinsic wave function, and the more difficult configuration-mixing matrix diagonalizations, which give physical wave functions, show that the rotational model of deformed nuclei is usable even when only a few valence particles are dynamically involved [2-6]).

With these wave functions, spectra are calculated that agree very well with experiments. However, the absolute energies of excited configurations and the matrix elements of electric operators do not come out well because these properties have a more essential dependence on the core wave function. It is not enough to consider just a few valence particles in computing these quantities.

The Nilsson model describes the core particles as well as the valence particles, and so it offers a method for the above problems. However, it is not clear that a simple model Hamiltonian will approximate the true Hamiltonian well enough to give similar wave functions. We shall calculate the core wave functions of several nuclei using a more realistic Hamiltonian, where the dynamics come from two-body interactions.

## 2. Description of the Core

The simplest many-particle wave function to write is the factorable form

$$\psi = \psi_v \phi_{\text{core}}.$$

Here $\psi_v$ is a few-particle intrinsic valence configuration, such as a two-particle two-hole or a four-particle four-hole excitation; $\phi_{\text{core}}$ is the wave function of all the rest

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of the particles. The Nilsson model wave function is of this form, and we shall similarly restrict the wave function. To calculate the total system energy, write

$$H = T + \sum_{ij} V(i,j), \tag{2.1}$$

$$\langle\psi|H|\psi\rangle = \langle\psi_{\mathrm{v}}|H|\psi_{\mathrm{v}}\rangle + \langle\phi_{\mathrm{core}}|H|\phi_{\mathrm{core}}\rangle + \sum_{ij}\langle\psi_{\mathrm{v}}(i)\phi_{\mathrm{core}}(j)|V(i,j)|\phi_{\mathrm{core}}(j)\psi_{\mathrm{v}}(i)\rangle. \tag{2.2}$$

The diagonal part of the last term is treated by defining a spherical potential well to hold the valence particles. The calculations in refs. [2-6]) then proceed by treating the first term realistically, allowing the valence particles to interact with each other via some two-body force.

If the valence particles are also allowed to polarize the core, there will be an additional gain in energy from the last two terms.

We shall neglect the change in $\psi_{\mathrm{v}}$ caused by the deformation of the core. This is reasonable because the polarization appears as a very slight change in the single particle orbitals and produces substantial energy changes only because many particles are involved. Since we consider only the intrinsic wave function, there are effects of projection which may shift the energy slightly. For example, a deformed core may give the total wave function a larger moment of inertia, or change the weights of the different angular momentum states within the intrinsic wave function.

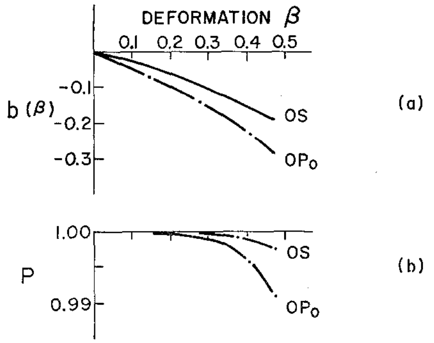

Fig. 1. Description of deformed harmonic oscillator orbitals in a spherical basis. (a) the amplitude of wave function two shells higher for deformed 0S and 0P orbitals, (b) the overlap probability of the deformed orbital with the spherical orbital plus the $2\hbar\omega$ excitation.

There are two points of departure for calculating the core wave function, depending on how much is assumed about the deformation. Using a harmonic oscillator well for the interaction, Nilsson found convenient a representation of the wave function where the single-particle orbitals are harmonic oscillator functions of variable axes. This makes an easily parametrized variational problem. The variational calculation has also been done with two-body forces [7,8]), but in this case it may be more economical algebraically to start with an orthonormal set of wave functions in a spherical basis. The single-particle orbitals are then characterized by a mixture of the spherical basis states, and a physical Hamiltonian may be diagonalized to find the mixture. Of course, the two procedures must be equivalent in the limit that the spaces of the wave functions spanned are the same.

The description of the deformed wave function in a spherical basis was first utilized to study how projection onto physical wave functions works in the degenerate Nilsson model $^{9}$).

It is useful to expand the single-particle orbitals of the degenerate Nilsson model in terms of spherical orbitals, to obtain some idea of what to expect with a more refined calculation. It is found that for low shells, to first order there is added only a component two shells higher. This description is good for quite large deformations. This may be seen from fig. 1, where the overlap probability $P$ for the 0S and 0P shells is plotted as a function of the deformation parameter $\beta$. Here

$$P = |\langle \chi_{\text{Nilsson}} | a\chi_{\text{s.m.}}(N) + \sum_{\alpha} b_\alpha \chi^{\alpha}_{\text{s.m.}}(N+2)\rangle|^2, \tag{2.3}$$

where

$$a(\beta) = \langle \chi_{\text{Nilsson}}(\beta) | \chi_{\text{s.m.}}(N)\rangle,$$

$$b_\alpha(\beta) = \langle \chi_{\text{Nilsson}}(\beta) | \chi^{\alpha}_{\text{s.m.}}(N+2)\rangle,$$

and $\chi^{\alpha}_{\text{s.m.}}(N+2)$ is a harmonic oscillator wave function of

$$E_0 = (N+2)+\tfrac{3}{2})\hbar\omega;$$

$\beta$ is related to the axes of the deformed wave function by

$$\left(\frac{b_x}{b_z}\right)^4 = \frac{1-\sqrt{5/\pi}\,\beta}{1+\frac{1}{2}\sqrt{5/\pi}\,\beta}.$$

This simple description would be reasonable also in perturbation theory; making the expansion

$$\chi_{\text{deformed}} = \chi_{\text{s.m.}}(N) - \frac{V_1}{T_1}\chi_{\text{s.m.}}(N+2) - \frac{V_2}{T_2}\chi_{\text{s.m.}}(N+4) + \ldots, \tag{2.4}$$

the higher components would have small coefficients in comparison to the first because of the large energy denominator and the smaller $V$ a reasonable hard-core force would provide $^{10}$).

At first sight the admixed wave function would have considerable freedom because of the $\frac{1}{2}(N+3)(N+4)$ degeneracy of the second higher shell, but it is restricted by parity considerations to three independent amplitudes. A requirement in typical variational calculations is that the nucleus retain the same overall volume under deformation, which further limits the wave function. This may be stated as a condition on the admixture of excited wave functions, that the particle and hole amplitudes be coupled to $L \neq 0$.

Two examples of volume-conserving deformed shells are

$$|0S'\rangle = (1+\alpha a_{\mathrm{d}}^{+} a_{\mathrm{s}})|0S\rangle,$$
$$|0P'\rangle = (1+\sum_{2,4} \alpha_L[a_{\mathrm{f}}^{+} a_{\mathrm{P}}]^L+\beta_2[a_{1\mathrm{P}}^{+} a_{\mathrm{P}}]^2)|0P\rangle. \tag{2.5}$$

As it stands, the first wave function will have a high overlap with a Nilsson wave function of some deformation depending on $\alpha$. The deformed 0P shell will approximate a Nilsson wave function only if restricted by $\alpha_4 = 0$, $\beta_2/\alpha_2 = \sqrt{\frac{4}{21}}$. The wave function derived from consideration of the two-body interaction will not necessarily satisfy this condition or even conserve volume. In fact, for some of the valence configurations the core will not be purely $S = 0$ and $T = 0$. Nevertheless, we expect deviations from the Nilsson form to be small.

The total wave function in the spherical basis is the Slater determinant of the product

$$\psi = \prod_{l} (a_i \chi(1)+b_i \chi'(i)). \tag{2.6}$$

This may be multiplied out and grouped into various terms depending on how many single-particle excitations a given part has. Thus

$$\psi = c_0 \psi_0+c_1 \psi_1+ \ldots, \tag{2.7}$$

where

$$c_n \psi_n = \sum_{\text{combinations}} \{\prod^{A-n} a_i \chi(i)\}\{\prod^{n} b_j \chi'(j)\}. \tag{2.8}$$

In the degenerate Nilsson model there are closed expressions for the coefficients $c_n$ (ref. [9])). We find that for light nuclei, such as $^{16}$O, it is quite satisfactory to use just the first two terms in the expansion. However, it may be seen from fig. 2 that for large deformations or the heavier nucleus $^{40}$Ca, this representation is inadequate.

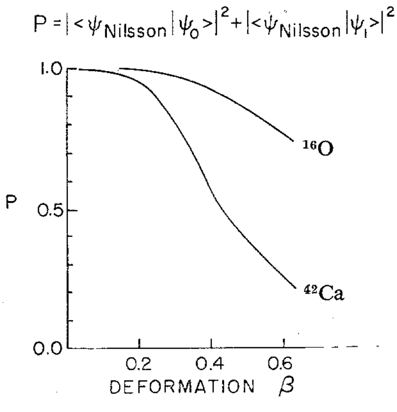

Fig. 2. Description of deformed wave function for $^{16}$O and $^{42}$Ca in a spherical basis, $\psi_0$ is the undeformed wave function and $\psi_1$ the wave function with $2\hbar\omega$ excitation.

If many terms have to be retained, the calculation will be unmanageably complicated. But the calculations for the individual orbitals are always relatively simple, and to a certain approximation, the single-particle excitations can be treated independently. Specifically, the approximation is that the diagonal energy of the part of the wave function with $n$ single-particle excitations is

$$\langle \psi_n | H | \psi_n \rangle = nT. \tag{2.9}$$

The error in this approximation is to have $\langle \psi_n | H | \psi_n \rangle$ too large for high $n$; this will make the core appear more rigid than it actually is.

The diagonal energy of $\psi_1$ is quite high. We use 25 MeV for oxygen and 19 MeV for calcium, but these values are not well determined †. Because the energy is so high, perturbation theory can be applied to find the amplitude admixtures for the single-particle orbitals.

## 3. The Calculation

We rewrite eq. (2.2) with the approximation that all of the two-body interaction in the Hamiltonian, except the off-diagonal core-valence interaction, has been taken into account by defining a spherical potential well and properly choosing the deformed valence wave function. We also treat the single-particle excitations as independent. Then

$$\langle H \rangle = E_{\text{valence}} + \prod_{i \text{ in core}} (a_i^2 + T b_i^2) + \sum_{i \text{ in core}} \langle [a_i \chi(i) + b_i \chi'(i)] \psi_\text{v} | V | [a_i \chi(i) + b_i \chi'(i)] \psi_\text{v} \rangle, \tag{2.10}$$

$\langle H \rangle$ will be minimized, when the $b_i$ are small, by the perturbation-theory value

$$b_i = -\frac{\langle \chi(i) \psi_\text{v} | V | \chi'(i) \psi_\text{v} \rangle}{T}. \tag{2.11}$$

For simplicity in the actual calculations, we take the valence state to be the leading U(3) state of maximum U(4) symmetry [4]. However, this gives a different

TABLE 1

Valence wave functions

| State designation | Number of valence particles | U(4), SU(3) quantum numbers |
|---|---|---|
| $^{16}$O* | 2p–2h | [4444] [ 4, 2] |
| $^{16}$O** | 4p–4h | [4444] [ 8, 4] |
| $^{18}$O | 2p | $[4^4\,2]$ [ 4, 0] |
| $^{18}$O* | 4p–2h | $[4^4\,2]$ [ 8, 2] |
| $^{40}$Ca* | 2p–2h | $[4^{10}]$ $[6, 0] \times [d^{-1}_{\pm 2})^2$ |
| $^{40}$Ca** | 4p–4h | $[12, 0] \times [d^{-1}_{\pm 2}]^4$ |
| $^{42}$Ca | 2p | $[4^{10}\,2]$ [ 6, 0] |
| $^{42}$Ca* | 4p–2h | $[12, 0) \times [d^{-1}_{\pm 2}]^2$ |

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† For further considerations on the excitation energy, see refs. [11,12]).

prescription than the Nilsson model for the holes in calcium wave functions, so for this case the orbital $d_{\pm 2}$ was used instead of the SU(3) orbital [0, 2]. The specific configurations are given in table 1.

A shortcoming of this calculation, which is present also in the Nilsson model, is that the wave function will contain some amplitude of a spurious state corresponding to centre-of-mass motion of the nucleus. The spherical closed shells form the SU(3) representation [0, 0]. When this is deformed, other representations are added. For a quadrupole deformation the representation [2, 0] is added, where the 2 corresponds to the creation operators

$$\sum_{i} (2a_z^+(i)a_z^+(i) - a_x^+(i)a_x^+(i) - a_y^+(i)a_y^+(i)), \tag{2.12}$$

acting on the closed shells. The spurious state, which is a two-quanta vibration of the entire nucleus, has the same SU(3) representation but with creation operators

$$\sum_{ij} (2a_z^+(i)a_z^+(j) - a_x^+(i)a_x^+(j) - a_y^+(i)a_y^+(j)). \tag{2.13}$$

The overlap probability between the two types of states is 0.07 for oxygen and practically negligible for the heavier calcium nucleus.

The calculation of two-body forces is facilitated by using harmonic oscillator wave functions for the single-particle orbitals, because then the wave function of the relative coordinate of two particles may be found explicitly. The S state forces will only act on the parts of the wave function with relative coordinate operator

$$[(a_x^+)^2 + (a_y^+)^2 + (a_z^+)^2]^N. \tag{2.14}$$

Calculation was done with the force used by Kallio and Kolltveit [13]), which is realistic enough to describe low-energy scattering and produce nuclear saturation, but which is still easy to compute with. For $^{16}$O, the oscillator constant of the wave function was chosen to be $\nu = 0.327$ fm$^{-2}$. For $^{40}$Ca we used $\nu = 0.27$ fm$^{-2}$. The constant $\nu$ is defined by $\nu = m\omega/\hbar$. The relative coordinate matrix elements were kindly supplied by Zamick and Mavromatis and are given for calcium in table 2.

TABLE 2

Matrix elements of the Kallio-Kolltveit force between states with harmonic oscillator relative wave functions

| | $\langle 0S\|V\|1S\rangle$ | $\langle 1S\|V\|2S\rangle$ | $\langle 2S\|V\|3S\rangle$ |
|---|---|---|---|
| $S = 0$ | −4.82 | −4.10 | −3.19 |
| $S = 1$ | −7.26 | −6.57 | −5.44 |

$\nu = 0.27$ fm$^{-2}$.

A technical problem arises in the calculations, to count the number of second-order interactions with a given permutation symmetry of the wave function. The second-order interaction is given in table 3, where $V$ denotes an interaction where a valence particle excites some core configuration, and $V'$ denotes the sum of the core-excitation matrix elements of a particle and a hole. Subscripts S, T denote singlet and triplet interactions. There is some ambiguity in these numbers, depending on how strictly the ansatz of factorable core and valence wave functions is maintained.

TABLE 3

Strength of core excitation with various valence wave functions

| Wave function | U(4) representation | Second-order interaction |
|---|---|---|
| 2-particle 2-hole | $[4^n]$ | $\frac{7}{2}(V'_T)^2+\frac{7}{2}(V'_S)^2+3V'_T V'_S$ |
| 2-particle $T = 1$ | $[4^n\,2]$ | $\frac{9}{2}V_T^2+\frac{5}{2}V_S^2+3V_T V_S$ |
| 4-particle 4-hole | $[4^n]$ | $9(V'_T)^2+9(V'_S)^2+18V'_T V'_S$ |
| 4-particle 2-hole $T = 1$ | $[4^n\,2]$ | $\frac{9}{2}(V_S^2+(V'_T)^2)+3(V_T V'_S+V'_T V'_S)$ $+\frac{5}{2}(V_S^2+(V'_S)^2)+6(V_T V'_S+V'_T V_S)+4(V_S V'_S)$ |

For example, the two-particle two-hole excitation of $[4^n]$ symmetry will be

$$\frac{1}{\sqrt{6}}(n\uparrow p\uparrow+n\uparrow n\downarrow+p\uparrow n\downarrow+p\downarrow n\downarrow+n\uparrow p\downarrow+p\uparrow p\downarrow).$$

A separate core wave function may be found for each term, or one core wave function may multiply this entire valence wave function.

TABLE 4

Core wave function of $^{42}$Ca*

| | $L = 0$ | | $L = 2$ | | $L = 4$ | | $L = 6$ | |
|---|---|---|---|---|---|---|---|---|
| | proton | neutron | proton | neutron | proton | neutron | proton | neutron |
| $gd^{-1}$ | | | −0.289 | −0.225 | +0.067 | +0.076 | −0.037 | −0.037 |
| $1dd^{-1}$ | +0.055 | +0.056 | −0.003 | −0.022 | +0.050 | +0.054 | | |
| $2sd^{-1}$ | | | +0.013 | −0.006 | | | | |
| $g1s^{-1}$ | | | | | +0.067 | +0.083 | | |
| $1d1s^{-1}$ | | | −0.079 | −0.072 | | | | |
| $2s1s^{-1}$ | −0.014 | −0.031 | | | | | | |
| $fp^{-1}$ | | | −0.247 | −0.180 | +0.048 | +0.059 | | |
| $1pp^{-1}$ | −0.031 | −0.052 | −0.031 | −0.037 | | | | |

The wave function is with Moshinsky's normalization of the harmonic oscillator orbitals [21]). The coefficients are the amplitudes of excitation of protons and neutrons of each spin.

There are several minor points which were taken into account in the calculation. The core excitation overlaps with the valence wave function, so the exclusion principle cuts down the normalization of the intermediate state. This effect is sensitive to the choice of valence wave function; it would be weaker had we used the Nilsson model instead of SU(3) valence wave functions. Also, when the valence wave function has holes, the core will not be the simple configuration of several closed shells.

Table 4 gives the core wave function of $^{42}$Ca calculated by perturbation theory. In accordance with our expectation, most of the strength is spin 2. The oxygen core wave functions are simpler since they only have amplitudes of $(0\mathrm{d}\,0\mathrm{s}^{-1})$, $(1\mathrm{s}\,0\mathrm{s}^{-1})$, $(0\mathrm{f}\,0\mathrm{p}^{-1})$, $(1\mathrm{p}\,0\mathrm{p}^{-1})$.

## 4. Comparison with Other Models

The intrinsic wave function will bear enough of a resemblance to the Nilsson prototype to make comparison useful. There is some value of the deformation parameter that will give the Nilsson wave function maximum overlap with the wave function calculated by the above method. In this way a deformation may be associated with the perturbation-theory wave function, even though it is too complicated to be described completely by this one number.

There are several other points of comparison of the variational and perturbative approaches. The variational plot of the system energy may be characterized by its curvature and the location of its minimum. This last tells us the equilibrium deformation and the energy gained by deforming. These quantities are of direct physical interest, being relevant to the E2 enhancements and position of the excitation spectra.

The curvature of the plot has a significance in vibrational models and may also be given an interpretation in our treatment. One may think of varying the wave function from the eigenstate that has been calculated, and compute the expectation value of $H$ and the equivalent deformation of the new state. If the eigenstate is

$$\phi_0 + c\phi_1,$$

with

$$\langle\phi_0|H|\phi_0\rangle \equiv E_0, \qquad \langle\phi_1|H|\phi_1\rangle = T,$$

then varying $c$, we have

$$\langle H\rangle = E_0 + T\left(\frac{\mathrm{d}c(\beta)}{\mathrm{d}\beta}\right)^2\beta^2 - \frac{\langle\phi_0|V|\phi_1\rangle^2}{T},$$

where $\beta$ is the equivalent deformation, defined by comparison with Nilsson wave functions. Thus the curvature of the Nilsson plot is proportional to the intermediate state energy with a factor to convert from the amplitude admixture representation to the deformation coordinate representation.

Table 5 shows the values of the curvature parameter used in various calculations. The hydrodynamic vibrational model estimates are the original ones of Bohr $^{14}$). Since these are derived from binding energy systematics, they are not expected to be valid for such light nuclei as are considered here.

To compare core deformations and energies in the Nilsson model and in perturbation theory, the equilibrium energy and deformation have been calculated in the

TABLE 5

Core deformability parameter D = $T(\mathrm{d}c/\mathrm{d}\beta)^2$

| | Nilsson | Perturbation theory | Hydrodynamic model |
|---|---|---|---|
| $^{16}$O | 37 | 43 | 15 |
| $^{40}$Ca | 91 | 114 | 23 |

TABLE 6

Comparison of core deformations

| Nuclear state | Nilsson | Perturbation theory |
|---|---|---|
| $^{16}$O* | $\beta = 0.34$ | $\beta = 0.31$ |
| $^{16}$O** | | 0.40 |
| $^{18}$O | 0.25 | 0.12 |
| $^{18}$O* | 0.37 | 0.34 |
| $^{40}$Ca* | 0.16 | 0.17 |
| $^{40}$Ca** | 0.34 | 0.28 |
| $^{42}$Ca | 0.08 | 0.10 |
| $^{42}$Ca* | 0.27 | 0.22 |

TABLE 7

Core contribution to system energy in MeV

| Nuclear state | Nilsson | Perturbation theory |
|---|---|---|
| $^{16}$O* | 4.5 | 4.25 |
| $^{16}$O** | 19 | 13.52 |
| $^{18}$O | 2.4 | 2.28 |
| $^{18}$O* | 12.8 | 8.90 |
| $^{40}$Ca* | 1.8 | 4.54 |
| $^{40}$Ca** | 9.2 | 14.68 |
| $^{42}$Ca | .5 | 2.10 |
| $^{42}$Ca* | 5.6 | 9.82 |

TABLE 8

Overlap probability of perturbation-theory core wave function with spherical core, and Nilsson core of optimum deformation

| State | Spherical | Nilsson |
|---|---|---|
| $^{16}$O* | 0.82 | 0.92 |
| $^{16}$O** | 0.51 | 0.81 |
| $^{18}$O | 0.92 | 0.96 |
| $^{18}$O* | 0.63 | 0.91 |
| $^{40}$Ca* | 0.78 | 0.94 |
| $^{40}$Ca** | 0.41 | 0.78 |
| $^{42}$Ca | 0.89 | 0.95 |
| $^{42}$Ca* | 0.55 | 0.85 |

Nilsson model by minimizing the Hartree-Fock energy,

$$\sum_i \{\tau_i(\beta)+\tfrac{1}{2}v_i(\beta)\}. \tag{2.15}$$

We use this in the form derived by Nilsson [1])

$$\tfrac{3}{4}\hbar\mathring{\omega}[\tfrac{1}{9}\sum_i (N_i+\tfrac{3}{2})\delta^2+\sum_i \kappa r_i(\delta)]. \tag{2.16}$$

Here $r_i(\delta)$ are the single-particle potential energies. The curvature parameter is just the kinetic part of eq. (2.16). Tables 6 and 7 compare the deformations and the core contribution to the system energy, respectively.

To give some measure of how much an improvement the Nilsson description of the core is over the spherical description, table 8 shows the overlap probability of the perturbed core with the spherical core and the Nilsson core of optimum deformation.

## 5. Conclusion

The calculation of deformations by perturbation theory allows one in principle to include effects which are outside the scope of other methods. For example, it is known that the effective potential well in saturating systems such as the nucleus must be velocity-dependent [15]), and this is accounted for by the proper choice of intermediate state energy. Also, the nucleon-nucleon force depends on $S$, $T$ and is strongly singular; the perturbation-theory treatment explicitly includes the $S$, $T$, dependence. But despite the different assumptions that go into the various models, there is quite good agreement on the energy of the core deformation.

The wave functions also give roughly the same E2 enhancements from core polarization. The effective charge from core polarization of the valence particles is about

$$e_{\text{core}} = 0.5,$$

both in perturbation theory [17]) and in the Nilsson model [16, 9]).

For nuclei with $T = 1$ valence wave functions, the core will have a considerable $T = 1$ component in perturbation theory but not in the deformed well models. This is because neutrons polarize the proton core more effectively than they polarize the neutron core. This point has also been discussed in relation to the effective E2 charge of valence particles [17, 18]).

In one respect the perturbation-theory wave function differs qualitatively from the variational wave function. There is a small but non-negligible volume change of the core, when particles are excited to make a more complicated valence configuration. In table 9 we have computed

$$\gamma = \frac{\langle\psi^*|\sum\limits_{\text{core protons}} r^2|\psi^*\rangle-\langle\psi|\sum\limits_{\text{core protons}} r^2|\psi\rangle}{\langle\psi^*|\sum\limits_{\text{valence protons}} r^2|\psi^*\rangle-\langle\psi|\sum\limits_{\text{valence protons}} r^2|\psi\rangle}. \tag{2.16}$$

Using the wave function of Brown and Green [19]) for the first excited state of $^{16}O$, a polarization of this magnitude is necessary to explain the strength of the experimentally observed monopole transition.

TABLE 9

Monopole polarization of core by valence wave function

| | |
|---|---|
| $^{16}O^*$–$^{16}O$ | $\gamma = 0.72$ |
| $^{18}O^*$–$^{18}O$ | 0.19 |
| $^{40}Ca^*$–$^{40}Ca$ | 0.60 |
| $^{42}Ca^*$–$^{42}Ca$ | 0.25 |

$\gamma$ = effective charge of valence particles from core deformation.

However, this polarization is the difference of the compressional polarization of the valence particles and the dialational polarization of the valence holes, and hence the amplitude is rather uncertain. Also, it has been found that off-diagonal matrix elements of $r^2$ are quite sensitive to the fringes of the wave function [18]). Therefore this estimate is not as reliable as the quadrupole deformation and energy calculations.

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