The realistic collective nuclear Hamiltonian

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The residual part of the realistic forces —obtained after extracting the monopole terms responsible for bulk properties— is strongly dominated by pairing and quadrupole interactions, with important $\sigma \tau \cdot \sigma \tau$, octupole and hexadecapole contributions. Their forms differ from the schematic ones through normalizations that lead to a universal $A^{-1/3}$ scaling for all multipoles. Coupling strengths and effective charges are calculated and shown to agree with the observed values.

21.60.Cs, 21.60.Ev, 21.30.xy

In the preceeding paper [1] the nuclear Hamiltonian was shown to separate into an “unperturbed” monopole field $H_m$ - that demands phenomenological treatment - and a “residual” multipole contribution, $H_M$, that is well given by existing realistic interactions [2,3]. In principle the task of fully characterizing $H$ becomes a pure monopole one, but for this characterization to be of practical use it is necessary to understand the structure of $H_M$, which is our present task.

It is through empirical evidence that we know that it must be possible to describe nuclei by solving the Schrödinger equation: the systems appear to be rather dilute - in the sense that the residual interaction is weak enough to be treated in perturbation theory - except for few (sub)shells in the vicinity of the Fermi level.

The quality of the interactions can be tested convincingly only in cases where exact diagonalizations are feasible in spaces large enough (typically one major shell) to ensure that what is left out can be treated perturbatively. The number of possible tests - though limited to vector spaces that do not exceed dimensionalities $O(10^7)$ - is significant, and it is certainly no accident that the realistic $H_M$ passes them all rather well. Therefore, the time may have come to trust the realistic forces rather than test them.

There are many advantages in doing so, but one is special. As new regions open to scrutiny - through Monte Carlo techniques [4] and further improvements in shell model technology [5] - the nature of the problems changes: Dimensionalities grow exponentially with the size of the systems, but the behaviour described by the enormous matrices also becomes simpler through the increasing influence of coherent effects.

The special advantage in trusting the Hamiltonian is that in adapting existing methods to face this situation, or designing new ones, our basic tool is the Hamiltonian itself.

It is here that a deeper understanding of $H_M$ is called for.

In section I we are going to show that its structure is as simple as could be expected, because of the strong dominance of pairing and lowest multipole operators. They appear in a normalized form that retains all the simplicity of their traditional counterparts but suffers none of their drawbacks.

In section II, it is explained how to ensure that a given choice of dominant terms is optimally extracted from the Hamiltonian.

Section III presents some estimates of the renormalizations due to core polarization effects.

Section IV is devoted to a comparison of different realistic interactions among themselves, and with the $W$ fit in the sd shell [6].

Appendix A contains results on the matrix defining the diagonal multipole representation.

Appendix B revisits the pairing plus quadrupole model.

I. DIAGONAL REPRESENTATIONS OF $H$

Our plan is as follows: a) Introduce $H_M$ in the two standard representations, b) reduce to sums of separable terms by diagonalization, c) show that the few dominant ones are normalized versions of the standard pairing and multipole forces, d) show that the normalizations are dictated by the universal $A^{-1/3}$ scaling for all couplings; and finally in e) say a few words about monopole the consequences of this result.

a) The Hamiltonian. We start by borrowing eqs. (I.41 to I.43) of [1] to write $H_M$ in the normal and multipole representations:

$$H_M = \sum_{r \leq s, t \leq u, \Gamma} W_{r s t u}^\Gamma Z_{r s t u}^\Gamma Z_{s t u}^\Gamma,$$

(1.1a)
\[ H_m = \sum_{rstu} \left[ \gamma \right]^{1/2} \frac{(1 + \delta_{rs})(1 + \delta_{tu})^{1/2}}{4} \omega_{rstu}^\gamma (S_{rt}^\gamma S_{su}^\gamma)^0, \]  

(1.1b)

\[ \omega_{rstu}^\gamma = \sum_{\Gamma} (-)^{s+t+\gamma-\Gamma} \left\{ \begin{array}{ccc} r & s & \Gamma \\ u & t & \gamma \end{array} \right\} W_{rstu}^\Gamma [\Gamma], \]  

(1.1c)

\[ W_{rstu}^\Gamma = \sum_{\gamma} (-)^{s+t+\gamma-\Gamma} \left\{ \begin{array}{ccc} r & s & \Gamma \\ u & t & \gamma \end{array} \right\} \omega_{rstu}^\gamma [\gamma], \]  

(1.1d)

Since \( H_m \) is defined as containing all the \( \gamma = 00 \) and \( 01 \) terms, \( H_M \) is defined by

\[ \omega_{rstu}^\gamma = 0 \text{ for } \gamma = 00 \text{ and } 01 \]

which explains the absence of one body contractions.

The normal or \( W \)-form is unique and the ordering of the indeces simply eliminates double counting: the contributions in \( rtsu,rstu,rsut \) and \( rust \) are identical, and it is just as well to keep only the first.

The multipole or \( \omega \)-form is highly non unique because the terms are not linearly independent and permuting indeces leads to different objects. We have chosen the variant in which summations are unrestricted for a reason that will become immediately apparent.

For the calculations we adopt the KLS force \([7,8]\), but in section IV the claim that the choice of realistic interaction does not matter much.

b) Separable form. We call \( H_m \) the restriction of \( \mathcal{H} \) to a finite set of orbits. Replacing pairs by single indeces \( rs \equiv x, tu \equiv y \) in (1) and \( rt \equiv a, su \equiv b \) in (2), and bringing the matrices \( W_{xy}^\Gamma \) and \( f_{ab}^\gamma = \omega_{ab}^\gamma \sqrt{(1 + \delta_{rs})(1 + \delta_{tu})}/4 \), to diagonal form through unitary transformations \( U_{zk}^\Gamma, u_{ak}^\gamma \):

\[
U^{-1}WU = E \rightarrow W_{xy}^\Gamma = \sum_k U_{zk}^\Gamma U_{yk}^\Gamma E_k^\Gamma
\]

(1.2a)

\[ u^{-1}fu = e \rightarrow f_{ab}^\gamma = \sum_k u_{ak}^\gamma u_{bk}^\gamma e_k^\gamma, \]

(1.2b)

and then,

\[
H_M = \sum_{k,\Gamma} E_k^\Gamma \sum_x U_{zk}^\Gamma Z_{x\Gamma} \cdot \sum_y U_{yk}^\Gamma Z_{y\Gamma},
\]

(1.3a)

\[
H_M = \sum_{k,\gamma} e_k^\gamma \left( \sum_a u_{ak}^\gamma S_a^\gamma \sum_b u_{bk}^\gamma S_b^\gamma \right)^0 \left[ \gamma \right]^{1/2},
\]

(1.3b)

which we call the \( E \) and \( e \) representations. Note here the explanation of the unrestricted ordering of the orbital indeces: it guarantees that in the \( f_{ab} \) matrices, \( a \) and \( b \) belong to the same set. In Appendix A it is explained what happens when they do not (asymmetric factorization).

c) Dominant terms. We have calculated the eigensolutions in (4) using KLS for spaces of one and two major oscillator shells. The density of eigenvalues (their number in a given interval) in the \( E \) representation is shown in fig. 1 for a typical two-shell case. It is skewed, with a tail at negative energies which is what we expect from an attractive interaction.

The \( e \) eigenvalues have a number of simple properties demonstrated in Appendix A: their mean value always vanishes, their width is \( \sqrt{1/8} \) of that of the \( E \) distribution, and they are twice as numerous. In fig. 2 we find that they are very symmetrically distributed around a narrow central group, but few of them are neatly detached. The strongest have \( \gamma = 1^{-0}, 1^{+1}, 2^{+0}, 3^{0}, 4^{0} \). If the corresponding states are eliminated from \( H \) in (4b) and the associated \( H \) in (4a) is recalculated, the \( E \) distribution becomes quite symmetric. Details will be given in section II, and here we only note that the residual skewness is entirely accounted for by the \( \Gamma = 1^{+0}, 0^{+1} \) and \( 2^{+0} \) peaks, of which the first remains strong at \( -7 \text{MeV} \).
This result is most telling because from the work of Mon and French we know that a symmetric $E$ distribution will lead to spectra in the $n$-particle systems that are identical to those of a random matrix. Therefore, we have found that - with the exception of three $\Gamma$ peaks - the very few dominant states in the $e$-distribution are responsible for deviations from random behaviour in $H_M$. Positively stated, these states are at the origin of collective properties.

If the diagonalizations are restricted to one major shell, negative parity peaks are absent, but for the positive parity ones the results are practically identical to those of figs. 1 and 2, except that the energies are halved, a striking feature whose significance will become clear soon.

In the list of important contributions whose structure we analyze we include the $\Gamma = 10$ and 01 terms, and the six strongest $\gamma$ ones

Their eigenstates (i.e. the factors in eqs.(4) with $k = 1$) will be compared with standard pairing and multipole operators. To fix ideas we write the form these eigenstates should take in the case of perfect pairing ($\Gamma = 01$) and quadrupole forces ($\gamma = 20$) acting in one shell of principal quantum number $p$. To compare with the result of a diagonalization, the operators must be normalized:

$$\mathcal{P}^+_p = \mathcal{P}^+_{01p} = \sum_{r \in p} Z^+_{rr01}/\Omega^{1/2}_{p}, \quad \Omega_p \cong 0.655 A_{mp}^{2/3}$$

$$\bar{q}_p \equiv M_{p}^{20} = \sum_{rs \in p} S_{rs}^{20} q_{rs}/\mathcal{N}_{p}, \quad \mathcal{N}_p^2 \cong 0.085 A_{mp}^{4/3}$$

where

- $\Omega_r = j_r + 1/2, q_{rs} = <r||r^2Y^2||s>/\sqrt{5}$
- $A_{mp}$ is the the total number of particles at midshell $p$ ($p^{(2)} = p(p - 1)$, remember)

$$A_{mp} = 2 \sum_{p' < p} (p' + 2)(2) + (p + 2)(2) = \frac{1}{3}(p + 1)(p + 2)(2p + 3) \approx \frac{2}{3}(p + 3/2)^3.$$

- the norms $\Omega_p$ and $\mathcal{N}_p$, are then

$$\Omega_p = \sum_r \Omega_r = \frac{(p + 2)(2)/2}{2} \approx \frac{1}{2}(3A_{mp}/2)^{2/3},$$

$$\mathcal{N}_p^2 = \sum q_{rs}^2 \cong 5(p + 3/2)^4/32\pi = \frac{5}{32\pi}(3A_{mp}/2)^{4/3}.$$

For the calculation of $\mathcal{N}_p^2$ we have used the matrix elements listed in (A11-15) of [1].

For the other strong multipoles the choice of operators is evident and for $\Gamma = 10$ the simple idea is that pairing in LS coupling should produce a good candidate. Labelling the orbits by their $\ell$ quantum numbers, we have two pairing terms

$$\mathcal{P}^+_ST = (\sum_{\ell} [\ell])^{-1/2} \sum_{\ell} [\ell]^{1/2} Z^+_{\ell\ell0ST} \quad ST = 01, 10,$$

which in $jj$ coupling become $\mathcal{P}^+_01 = \Omega_p^{-1/2} \sum_r \sqrt{\Omega_r} Z^+_{rr01}$

$$\mathcal{P}^+_10 = \Omega_p^{-1/2} \sum_{jj'} [\ell]^{1/2} (\ell\ell)0 (1/2 1/2)1 (jj')1 Z^+_{jj'10},$$

where we have recovered the usual $r \equiv j\ell$ label, and used a self evident notation for the LS to $jj$ transformation. In table I these operators are compared with the results of the diagonalization. It is apparent that $\mathcal{P}^+_01$ accounts very well for $(U^0_{jj})_p$. For $\mathcal{P}^+_10$ vs $(U^1_{jj})_p$ the agreement is not so excellent, but still good. The overlaps are found under $< U_p | P >$ in table II, which also contains the corresponding values of $< u_p | M >$ for the lowest multipole operators $M$. The agreement is again excellent except for the $\sigma$ case, for which it is only fair. Note that the form of these operators is given in the Appendix of [1].
TABLE I. Eigenvectors and energies calculated in the $pf(p=3)$, $sdg(p=4)$, and $pf + sdg(3+4)$ spaces compared with the normalized pairing operators $\bar{P}_{10}$ and $\bar{P}_{01}$

| $\bar{P}_{10}$ | $(U^r_{10})_{3,4}$ | $\sqrt{2}(U^r_{10})_{3+4}$ | $\bar{P}_{01}$ | $(U^r_{01})_{3,4}$ | $\sqrt{2}(U^r_{01})_{3+4}$ |
|----------------|------------------|------------------------|----------------|------------------|------------------------|
| 77            | -.65             | -.65                   | -.66           | .41              | .31                    |
| 75            | -                | -                      | -.68           | .31              | -.74                   |
| 33            | -.45             | -.38                   | -.41           | .33              | .26                    |
| 35            | 0.               | 0.                     | 0              | .33              | -.30                   |
| 31            | -                | -                      | .42            | -.30             | .43                    |
| 55            | -.55             | -.58                   | -.59           | -.27             | -.12                   |
| 11            | -.32             | -.29                   | -.31           | -.04             | .07                    |

$E_{\Gamma(3)}$ | -2.95 | -4.59 |

| $\bar{P}_{01}$ | $(U^r_{01})_{3,4}$ | $\sqrt{2}(U^r_{01})_{3+4}$ | $\bar{P}_{10}$ | $(U^r_{10})_{3,4}$ | $\sqrt{2}(U^r_{10})_{3+4}$ |
|----------------|------------------|------------------------|----------------|------------------|------------------------|


TABLE II. Energies and eigenstates of the dominant terms ($\gamma = 21$ added for illustrative proposes). See text.

| $\gamma$ | $c_3^+$ | $c_4^+$ | $c_{3+4}^+$ | $M$ | $<u_3|u>|u_3'|u_3''>$ | $<u_4|u>|u_4'|u_4''>$ | $<u_3|u_1'>u_3''>$ | $<u_4|u_2'>u_4''>$ | $\alpha^2$ |
|----------|--------|--------|-------------|-----|----------------|----------------|----------------|----------------|-------------|
| 11       | 1.77   | 2.01   | 3.90        | $\sigma\tau$ | .992 | .994 | .999 | 1.000 | .94          |
| 20       | -1.97  | -2.14  | -3.88       | $r^2Y_2$     | .996 | .997 | 1.000 | 1.000 | .95          |
| 10       | -1.02  | -0.97  | -1.96       | $\sigma$     | .880 | .863 | .997 | .994 | 1.04         |
| 21       | -0.75  | -0.85  | -1.60       | $r^2Y_2\tau$ | .991 | .998 | .999 | .997 | .94          |

| $\Gamma$ | $E_{3}^\chi$ | $E_{4}^\chi$ | $E_{3+4}^\chi$ | $P$ | $<U_3|P>|U_3|P>$ | $<U_4|P>|U_4|P>$ | $<U_3|U_3'>|U_3''>$ | $<U_4|U_4'>|U_4''>$ | $\alpha^2$ |
|----------|--------------|--------------|-----------------|-----|----------------|----------------|----------------|----------------|-------------|
| 01       | -2.95        | -2.65        | -5.51           | $P_{01}$ | .992 | .998 | 1.000 | .994 | 1.048       |
| 10       | -4.59        | -4.78        | -10.12          | $P_{10}$ | .928 | .910 | .998 | .997 | .991        |
Interesting as these results might be, the truly remarkable ones come when we diagonalize in two major shells. Let us go back to table I, and note that the eigenstates can always be written as

$$U_{3+4} = (\alpha U_A + \beta U_P)/\sqrt{2} \quad \alpha^2 + \beta^2 = 2,$$

(1.7)

where $U_p'$ can - in principle - be any unit vector, but in fact it is almost identical to $U_p$. This is always the case as table II shows: $< U_i U_i' >$ and $< u_i u_i' >$ are strikingly close to 1 with no exceptions while $\alpha^2$ is quite close to 1.

Therefore, for any normalized pairing or multipole operator $O$ we have that

If $O_p$ and $O_{p+1}$ are eigenstates for shell $p$ and $p+1$ separately, then $(O_p + O_{p+1})$ is very much the eigenstate for the space of the two shells. The eigenvalues are very close in the three cases.

Note that we have chosen a normalization of 2 for the two shell eigenstates so as to halve its eigenstate.

Before we examine the consequences of this result, we mention a few facts about the other contributions.

In table II we have added the $\gamma = 21$ case as a reminder that isovector multipoles are always present. Their strength is between 30 and 40% of that of the isoscalar terms (precise numbers are given in table III in section II) and they have identical structure.

The dominant negative parity contributions are

- $\gamma = 10$ at 4.59 MeV, $< rY^1_0 | u^{10} > = 0.994$
- $\gamma = 30$ at 2.69 MeV, $< rY^3_0 | u^{30} > = 0.986$

The first is a center of mass operator. Its presence simply reflects the translation invariance of the interaction. Its $\gamma = 11$ counterpart, associated to the giant dipole resonance (GDR), comes at 1.81 MeV. The other strong term is responsible for octupole collectivity. (In deciding whether a given multipole is attractive or repulsive it should be remembered that $(M^* M^*)^0 = (-\gamma^3)^{-1/2} (M^* M^*)$).

**d) Universal scaling.** We have now the necessary elements to construct a schematic but accurate collective Hamiltonian. From [3] we know that

$$W_{xy}^T(\omega) \cong \frac{\omega}{\omega_0} W_{xy}^T(\omega_0)$$

(1.8)

and therefore the eigenvalues in table II must scale in the same way. Setting $\alpha^2 = 1$ in eq.(1.7) for simplicity, the normalized pairing and quadrupole forces become

$$H_p = -\frac{\hbar \omega}{\hbar \omega_0} |E^{01}| (\bar{P}_p + \bar{P}_{p+1}) \cdot (\bar{P}_{p} + \bar{P}_{p+1})$$

(1.9)

$$H_q = -\frac{\hbar \omega}{\hbar \omega_0} [e^{20}] (\bar{q}_p + \bar{q}_{p+1}) \cdot (\bar{q}_p + \bar{q}_{p+1})$$

(1.10)

which we take as representative of the “collective” Hamiltonian because of their known coherence. For the other strong terms the expressions are strictly similar, and all arguments concerning pairing and quadrupole expressions apply to them. Since $e_1^0 \cong e_2^0 \cong e_3^0 / 2$ (same for $E^\gamma$), the coupling constants could be taken to be independent of the space chosen; which may be any of the shells or the two together.

The term normalized applies to the one shell operators. For two or more shells it is more convenient not to normalize their sum, since it is in this form that the couplings are constant.

Equations (1.9) and (1.10) call for a generalization to an arbitrary number of shells and it does not take much imagination to discover what it should look like. However it is interesting to understand the origin of this very welcome simplicity. Let us start from the obvious it is always possible to write the lowest state associated to multipole $\gamma$ as $\sum O^{(\gamma)}_p / N^{(\gamma)}_p$.

To say something rigorous about the radial form of $O^{(\gamma)}_p$ does not seem trivial, but granted that it is close to the multipole operator in shell $p$, then $N^{(\gamma)}_p$ is fixed by a scaling argument.

In leading order the expectation value of a Hamiltonian must go as the number of particles in the system. Therefore, in $H$, the leading monopole terms must go as $O(A)$, and $H_M$ acting on one shell must go at most as $O(D = O(A^{2/3}))$, where $D$ is the degeneracy of the Fermi shell. Since there are $p$ possible contributors, each individual multipole term must go as $O(A^{1/3})$.

It is precisely what the normalized operators ensure, given the universal scaling provided by the $\hbar \omega$ factor.

In our particular cases: $n$ particles in shell $p$ can produce an energy proportional to $nD$ for the pairing, and $n^2D$ for the quadrupole forces, which the normalizations reduce to $n$ and $n^2/D$. Since $n = O(D) = O(A^{2/3})$, when multiplied
by \( \hbar \omega = O(A^{-1/3}) \) both contributions become \( O(A^{1/3}) \). If the \( n \) particles are promoted to some higher shell with \( p = p + M \), there is no pairing gain, a slight quadrupole loss and a monopole loss \( O(M \omega) \) that remains \( O(A^{1/3}) \) as long as \( M \) is not too large.

For the conventional pairing and quadrupole forces the energies in one shell would be \( nD/A \) and \( n^2D/A^{5/3} \) respectively, as their scalings are chosen to yield the correct \( O(A^{1/3}) \) magnitude. But now when the particles are promoted \( D \rightarrow (p + M)^2 \), and not only there is a gain: it becomes larger than the monopole loss that is only linear in \( M \) and the system collapses. If the forces are restricted to act in finite spaces, to obtain sensible results the coupling constants must be reduced as the space is increased. (The problem will be discussed in Appendix B).

The normalization is defined only to leading order \( O(p^k) \), and we can say nothing about the \( O(p^{k-1}) \) terms, responsible for \( \alpha^2 \neq 1 \), and the slight differences we have neglected in the \( e \) and \( E \) couplings, but this is the good reason to neglect them.

What the argument does not explain is why the pairing and multipole operators in one shell resemble their ideal counterparts as closely as we have found so far. There is a hint, however, in that they must be the ones capable of producing coherence. More on this on the next subsection, and in section III, it will be shown that the \( g'_p \) that couples shell \( p \) to \( 2\hbar \omega \) jumps, remains indeed close to \( q_p \).

We have found therefore, that we can recover the geometrical simplicity of the pairing plus quadrupole model without its fundamental flaw: the space dependence of the coupling constants. The model has an enormous historical interest, and it is very instructive to show how far we can go in justifying it (see Appendix B).

e) The monopole hint. If \( \mathcal{H}_M \), is as good as we have argued why not trust the information it can provide about \( \mathcal{H}_m \)? It is quite possible that, rather than wrong, it is only insufficient and its study is most interesting.

As befits the leading term in a multipole expansion, the monopole one is the strongest: in fig. 2 it would come at \(-10 \text{ MeV}\). Unsurprisingly it has the form \( \sum n_p/\sqrt{D_p} \), which is what we expect of normalized operators, but it should be mentioned that there are several monopole candidates one can think of: 1, which is the \( \hat{n} \) operator in second quantization; but also \( \hat{r} \) for instance. When normalized they give the same result.

The remarkable thing about this form is that it provides the answer to the problem raised at the end of the preceeding paper. Which is that \( \hat{n} \), suffers from the defect of the conventional separable forces in that it must be associated with a coupling constant that is space dependent. There is no collapse now because \( n \) is a conserved quantity, and an \( A^{-1} \) scaling ensures the asymptotically correct behaviour and the coupling tends to a constant. Contrary to the pairing and quadrupole cases there can be no energetic gain in promoting particles to higher orbits but there is no loss either, and this is a subtle form of collapse because a good Hamiltonian \textit{must} ensure the existence of a Fermi level, i.e., it must force the particles to occupy the lowest orbits. The normalized monopole operator does it by producing a discontinuity at each shell closure. Therefore, it is not only responsible for the bulk energy of nuclear matter, but it also takes care of the major shell effects.

This operator suggests the starting point in the construction of \( \mathcal{H}_m \). For a preliminary attempt see \([23]\), where a mass formula - of rather high precision by present standards - is derived.

II. CHOICE AND COMPLETE EXTRACTION OF \( H_C \)

The choice of \( H_C \). The results so far invite a separation:

\[
H = \mathcal{H}_m + H_C + H_R
\]

where \( H_C \) is the collective or coherent part, while \( H_R \) is the rest. To define them with some precision, we shall rely on the result of Mon and French \([9]\) that \( H_R \) could be viewed as random, as soon as its \( E \) distribution becomes symmetric.

The distributions will be characterized by their moments:

\[
m_k = \frac{2}{D(D - 1)} \sum E_k^k, \quad \gamma_3 = m_3/m_2^{3/2}
\]

and the vanishing of the skewness \( \gamma_3 \) will be seen to be sufficient to ensure symmetry. We use \( m_2 = \sigma^2 \).

Let us then define some cut off \( \varepsilon \), eliminate from \( H \) in the \( e \) representation those states with \( |e_\varepsilon| > \varepsilon \), and decrease \( \varepsilon \) until the \( E \) distribution becomes symmetric. The result of the operation is shown in figs. 3, 4 for \( \varepsilon = 2 \) and 1.3 MeV respectively. Labelling the original distribution in fig. 1 as \( (\varepsilon = \infty) \), we find the following moments \( (\sigma^2 \text{ in MeV}) \).
TABLE III. The $sdg + pf$ states in the $f$-representation ($|e_γ| > 1.3$) and their $pf$ and $sdg$ counterparts. $S^x, A^x =$ symmetry type and parity. $↑$ signals the states singled out in fig.2, and their one shell counterparts. $↓$ is for states with $|e_γ| < 1.3\text{MeV}$ that are likely to have a clear multipole character. Parenthesis indicate that the assignment is unchecked but given as plausible.

| $\lambda\tau$ | sym  | type     | $e_{pf, sdg}$ | $e_{pf}$ | $e_{sdg}$ |
|---------------|------|----------|---------------|----------|----------|
| $00$          | $A^-$| $\ldots$ | $1.88$        | $\ldots$ | $\ldots$ |
| $10$          | $S^-$| $r_1Y_1$ | $4.59$        | $\ldots$ | $\ldots$ |
|               | $S^+$| $\sigma$ | $-1.96$       | $\ldots$ | $-1.02$  |
|               |      | $\ldots$ | $-1.53$       | $\ldots$ | $-0.97$  |
|               |      | $\ell$   | $1.44$        | $0.66$   | $0.80$   |
|               | $S^-$| $\ldots$ | $1.41$        | $\ldots$ | $\ldots$ |
| $11$          | $S^+$| $\sigma\tau$ | $3.90$ | $\ldots$ | $1.77$  |
|               |      | $\ldots$ | $-1.83$       | $\ldots$ | $-2.01$  |
|               |      | $r_1Y_1\tau$ | $1.81$ | $\ldots$ | $\ldots$ |
| $20$          | $S^+$| $r^3Y_2$ | $-3.88$       | $\ldots$ | $-1.97$  |
|               |      | $\ldots$ | $1.31$        | $0.64$   | $0.75$   |
| $21$          | $S^+$| $r^3Y_2\tau$ | $-1.60$ | $\ldots$ | $-0.75$  |
|               |      | $M2??$   | $-1.55$       | $\ldots$ | $-0.85$  |
|               | $A^+$| $\ldots$ | $1.46$        | $0.64$   | $0.76$   |
| $30$          | $S^-$| $r^3Y_3$ | $2.69$        | $\ldots$ | $\ldots$ |
| $31$          | $S^-$| $r^3Y_3\tau$ | $1.14$ | $\ldots$ | $\ldots$ |
| $40$          | $S^+$| $(r^4Y_4)$ | $-2.11$       | $\ldots$ | $-1.12$  |
| $41$          | $S^+$| $(r^4Y_4\tau)$ | $-0.91$ | $\ldots$ | $-1.24$  |
| $50$          | $S^-$| $(r^5Y_5)$ | $1.75$        | $\ldots$ | $\ldots$ |
| $51$          | $S^-$| $(r^5Y_5\tau)$ | $0.78$ | $\ldots$ | $\ldots$ |
| $60$          | $S^+$| $(r^5Y_6)$ | $-1.26$       | $\ldots$ | $-0.73$  |
|               |      | $\ldots$ | $\ldots$     | $\ldots$ | $-0.82$  |
• \( \varepsilon = \infty \quad \sigma^2 = 0.99, \quad \gamma_3 = -2.22. \)

Since the lowest state \( \Gamma = 1^+0 \) is at \(-10.12 \text{ MeV}\) its contribution to \( \gamma_3 \) is by far the largest but still only \(-0.61.\)
It means that many states in the tail must contribute to \( m_3. \)

• \( \varepsilon = 2.0 \quad \sigma^2 = 0.60, \quad \gamma_3 = -0.79. \)

Five peaks have been excluded \( \gamma = 1^-0, 1^+1, 2^+0, 3^-0 \text{ and } 4^+0 \) and now the \( \Gamma = 1^+0 \) state at \(-7.79 \text{ MeV}\)
accounts for most of \( \gamma_3 \) with a contribution of \(-0.60,\) which when added to that of the next two states \( \Gamma = 2^+0 \)
\((-4.29 \text{ MeV}) \) and \( 0^+1 \) \((-3.82 \text{ MeV}), \) at \( \gamma_3 = -0.86,\) exceeds the full value. As anticipated, the very large \( e \) states
are responsible for most of the tail of the original distribution. Although distortions are still apparent, they may
be interpreted as fluctuations and we have a good model for \( H_C \equiv \) the five \( \gamma \) states and the \( \Gamma = 1^+0, 0^+1 \) ones.

Since it is not only the size, but also the ability to generate coherence that must characterize the main terms
we have left out \( \Gamma = 2^+0 \) which - as we shall see in section IV - must be counted as a nuisance, rather than a
bona fide candidate to \( H_C. \)

It should be noted that the structure of the large \( \Gamma \) states is little changed in going from \( \varepsilon = \infty \) to \( \varepsilon = 2. \)

• \( \varepsilon = 1.3 \quad \sigma^2 = 0.41, \quad \gamma_3 = -0.002 \)

This cut-off was chosen as a sensible definition of the bulk of the \( e \) distribution. The histogram in figure 4 now
becomes structureless. The \( \gamma \) states with \( |e_\gamma| > 1.3 \) are listed in table 3. Some useful information is given, as
their symmetry type (see eqs. (1.30-32) in [1]), and their multipole nature whenever possible.

The cut off is reasonable in that the majority of excluded states belong naturally to what is expected from a
multipole decomposition. However, several peaks have an ill defined status, while others we would include in \( H_C \) have
missed the cut off (e.g. \( 3^-1 \) at \( e = 1.14.\) Clearly we are in the boundary where the small terms in \( H_C \) overlap the
large ones in \( H_R. \)

Two attitudes compete in choosing \( H_C: \) Include either as much as necessary or as little as possible. Which one is
given precedence depends on the computational strategy adopted.

As much as necessary applies to the recently developed shell model Monte Carlo approach [4]. The Hamiltonian
must be written in some \( e \) representation, and the authors have chosen an ingenious one in which they introduce the
Pauli violating terms necessary to cancel all \( \gamma = \lambda_1 \) terms. To understand how it can be done refer to eq.(1.47b)
in the preceding paper[1], and imagine that in \( V^{JT}_{rstu} \) the \( rs \) and \( tu \) states are allowed to be symmetric. Since the
purpose of the exercise is to reduce the number of terms, it is probably a good idea to proceed as we have done and
choose a proper \( H_C. \) The problem is that pairing has to be included in the \( e \) representation which may be costly, but
an example given at the end of the section suggests that the cost is probably not too high.

As little as possible, can be reconciled with as much as necessary by treating first the truly important terms and
then doing some form of perturbation theory to account for the rest. Here pairing plus quadrupole or even only one of
them may be sufficient.

One example may be mentioned. In a forthcoming study [1], it is shown that states of 4 neutrons and 4 protons
moving in the same or contiguous major shells, generate rotational spectra exhibiting systematic backbending. With a
proper \( \hat{\varepsilon} \cdot \hat{q} \) the wavefunctions have overlaps of better than 0.95 with those of the realistic interaction \( H, \) but the
backbending has gone. However when the expectation value of the full \( H \) was calculated using the \( \hat{\varepsilon} \cdot \hat{q} \) eigenstates, the
spectrum reproduces perfectly the exact one: lowest order perturbation theory may work very well with a reasonably
good starting vector.

This example is particularly relevant because the “proper” quadrupole that reproduces best the exact results is
some 30% larger than \( e \) eigenvalue in table 3. It is probable that part of the effect is due to the isovector quadrupole
that was not included in the calculation. But there is another cause as we see next.

Complete Extraction

\( H_C \) and \( H_R \) in the normal representation, can be thought as vectors, each matrix element \( W^T_{rstuC} \) and \( W^T_{rstuR}, \) being associated \([\Gamma]\) to unit vectors. Then the norm is simply \( m_2 \equiv \sigma^2 \) (assume in all that follows that the matrix
elements have been all divided by \( D(D+1)/2 \))

\[
\sigma^2 = \langle (H_C + H_R)^2 \rangle = \sum (W^T_{rstu})^2 [\Gamma] \\
= \sum [(W^T_{rstuR})^2 + (W^T_{rstuC})^2 + 2W^T_{rstuR}W^T_{rstuC}] [\Gamma] \\
= H_C^2 + H_R^2 + 2H_C \cdot H_R \\
(2.1)
\]
It is elementary to show that if \( H_1 \) and \( H_2 \) are the Hamiltonians associated to eigenvectors \( E_1 \) and \( E_2 \), then 
\[
< H_1 H_2 > = H_1 \cdot H_2 = 0.
\]

The crux of the matter is that \( H_C \) and \( H_R \) are by construction orthogonal in the multipole representation, but they need not be in the normal one. We may even invent vectors orthogonal in the former that become parallel in the latter. This, because of the non linear independence problem encountered several times in [1]: a multipole decomposition can teach us what to separate, but not how to separate.

What has been done in the preceding section illustrates quite well the first part of the proposition, and incidentally the need to use the \( f \) matrix elements in eqs.(1.2), to ensure symmetric factorizations, since any other choice would have led to opaque results. Now that we know what to separate, we should do it well.

The simplest way is to write 
\[
H_R + H_C = \left( H_R - \frac{H_C \cdot H_R}{H_C \cdot H_C} H_C \right) + H_C \left( 1 + \frac{H_C \cdot H_R}{H_C \cdot H_C} \right),
\]
which makes the two terms orthogonal. By squaring we find
\[
\left[ H_R^2 - \frac{(H_C \cdot H_R)^2}{(H_C \cdot H_C)} \right] + \left[ H_C^2 + 2H_C \cdot H_R + \frac{(H_C \cdot H_R)^2}{(H_C \cdot H_C)} \right]
\]
and since \( \frac{(H_C \cdot H_R)^2}{(H_C \cdot H_C)} \) can be safely neglected, the orthogonalization amounts to leave \( H_R \) almost untouched, and to boost \( H_C \) by the cross term. Now we call upon eq. (A6), which says that the total norms in the two representations are
\[
\text{sd}
\]
and therefore
\[
\text{sd} = 0.70, \text{ and therefore the orthogonalization boosts the share of } H_C \text{ to 40\%, which implies a } \sqrt{4/3} \approx 15\% \text{ increase in the coupling constants.}
\]

This should be sufficient to have an idea of the effect, but for a quantitatively reliable extraction, each term must be treated separately. Let us see how.

Assume we have selected the candidates to \( H_C \), transformed to the normal representation the multipole ones, and made them monopole free. Call them \( H_\kappa \). We want to find the linear combination \( H_C = \sum C_\kappa H_\kappa \), that maximizes the overlap between \( H_C \) and \( H \). It amounts to solve the standard problem (\( \alpha \equiv rstu \))
\[
\sum_\alpha (W_\alpha^T - \sum_\kappa C_\kappa W_{\alpha\kappa}^T) [\Gamma] = (H - \sum_\kappa C_\kappa H_\kappa)^2
\]
\[
= H \cdot H - 2 \sum_\kappa C_\kappa H_\kappa \cdot H + 2 \sum_{\kappa,\kappa'} C_\kappa C_{\kappa'} H_\kappa \cdot H_{\kappa'} = \min
\]
(2.2)
and therefore \( C_\kappa \) is determined by the linear system
\[
H_\kappa \cdot H = \sum_{\kappa'} H_\kappa \cdot H_{\kappa'} C_{\kappa'} \quad (2.3)
\]

The \( H_\kappa \) vectors can be made orthogonal by diagonalizing the norm matrix \( H_\kappa \cdot H_{\kappa'} \) through transformation \( T_{\mu\nu} \)
\[
H_\mu = \sum T_{\mu\kappa} H_\kappa, \quad H_\kappa = \sum T_{\kappa\mu} H_\mu; \quad H_\mu \cdot H_{\mu'} = \delta_{\mu\mu'} H_\mu^2. \quad (2.4)
\]
Therefore, defining \( H_C \) in terms of the \( H_\mu \), we have
\[
H_C = \sum C_\mu H_\mu \quad (2.5)
\]
As we see the analysis in the first section has fulfilled its part in pointing to the correct forms to be extracted, but the associated coupling constants may need some corrections. If our estimates are correct, they should not exceed 20%.

It is worth emphasizing that once the fully extracted \( H_C \) is transformed back to the multipole representation it may look quite different from the original, which is not monopole free, and contains Pauli violating terms. However, it is very much the original.

A potentially useful variant of this possibility was found in the \( sd \) shell: When the strongest contribution for each \( \gamma \) is included and extraction is carried maximizing the overlap, the addition of the pairing term makes no difference.
III. CORE POLARIZATION

To account for the effect of states outside of one or two major shells in which we are prepared to work, we use the quasiconfiguration method [12,13]. The idea is to separate the full space into a model space containing states \(|i\rangle\) and an external one made of states \(|j\rangle\). The \(|i\rangle\) and \(|j\rangle\) states are now “dressed” through a transformation that respects strict orthogonality

\[ |\bar{i}\rangle = |i\rangle + \sum_j A_{ij} |j\rangle \]

\[ |\bar{j}\rangle = |j\rangle - \sum_i A_{ij} |i\rangle \]

\[ <i|H|j> = 0 \]

The amplitudes \(A_{ij}\) are then defined by

\[ <\bar{i}|H|\bar{j}>=0 \]

Perturbation theory is the natural way to determine \(A_{ij}\), since whatever must be treated exactly is in principle contained in the model space, which we take here to be a full shell \(p\). What is nice about the quasiconfiguration method, is that it makes it very clear how the dressing of the states is transformed into the dressing of the operators.

We refer for details to [12,13], from which we borrow the expression for the second order correction, and apply in some detail to the pairing, and quadrupole Hamiltonians.

**Pairing.** We deal first with the effect of shell \(p+1\) only. \(E_{01}\) is a one shell energy from table 2, scaled by \(\hbar\omega/\hbar\omega_0\), and \(\hbar\omega_0 = 9\text{MeV}\).

\[ <i|H_P|i'> = <i|E_{01}(\omega)\frac{P^+_p \cdot P_p}{\Omega_p}|i'> \]

\[ -\frac{E_{01}^2(\omega)}{2\hbar\omega} \sum_j <i|P^+_p \cdot P_{p+1}|j><j|P^+_p \cdot P_p|i'> \frac{1}{\sqrt{\Omega_p \Omega_{p+1}}\sqrt{\Omega_p \Omega_{p+1}}} \]

\[ = <i|E_{01}(\omega)\frac{P^+_p \cdot P_p}{\Omega_p} - \frac{E_{01}^2(\omega)}{2\hbar\omega} \frac{1}{3} \frac{P^+_p \cdot P_p \cdot P_{p+1}^+ \cdot P_{p+1}}{\Omega_p \Omega_{p+1}}|i'> \]

\[ <i|E_{01}(\omega)\frac{1}{2} \left( 1 - \frac{E_{01}(\omega)}{4\hbar\omega_0} \right) \frac{P^+_p \cdot P_p}{\Omega_p}|i'> \]

Step by step we find

a) the unperturbed energy, to which we add

b) the second order perturbation. The intermediate states are assumed to be all at energy \(2\hbar\omega\). Then

c) invoking closure and recoupling the operators (hence the factor 1/3),

d) the final result follows by contracting out the the operators in shell \(p+1\) (which gives back a factor 3).

Repeating the operation to account for states in shell \(p-1\) leads to exactly the same correction and we conclude that the renormalized operator is the original one affected by a modified \(E_{01}\)

\[ E_{01} \rightarrow E_{01}(1 + \frac{|E_{01}(\omega)|}{\hbar\omega}) \equiv E_{01} \rightarrow E_{01}(1 + 0.32), \]

(3.2)

Now consider what would happen if we were to generalize to an indefinite number of shells, and compare with the result for ordinary pairing:

\[ E_{01}(\omega) \rightarrow E_{01}(\omega) \left[ 1 + \frac{|E_{01}(\omega)|}{2\hbar\omega} \left( 1 + \frac{1}{2} + \frac{1}{3} + \cdots \right) \right] \]

\[ G \rightarrow G \left[ 1 + \frac{|G|}{2\hbar\omega} \left( \frac{\Omega_{p+2}}{2} + \frac{\Omega_{p+3}}{3} + \cdots \right) \right]. \]

(3.3)

(3.4)

The normalization of the operators \(P_p\) transforms a bad divergence into a logarithmic one. Since high lying pairing excitations violate badly translation invariance the corresponding matrix elements should be quenched, and this
is probably sufficient to eliminate the divergence. Plausible as this argument may be, the fact remains that the renormalization of the pairing force is a delicate problem that has yet to be solved. Some more on this at the end of the section.

**Quadrupole.** The problem of multipole renormalizations is very different from the one we have analyzed for pairing because the physical processes are different. Where we had two particles jumping to higher shells, or being promoted from lower ones, now it is a particle-hole excitation that is produced by the valence particles, and it is in the multipole representation that the problem is naturally treated, and the space involved is always finite in second order for the operators of interest.

In particular, the quadrupole renormalization are due to $2\hbar\omega$ jumps mediated by a term of the form $k(q'_p \cdot \tilde{q}_{2h\omega} + \tilde{q}^*_p 2h\omega \cdot \tilde{q}_p)$, which must be extracted from $H_{Hf}$. The primes indicate that the operators may not be genuine quadrupoles. The extraction method is a variant of the diagonalizations we have used so far. It is explained in Appendix A under the item asymmetric factorization. The space involves all shells from $p = 0$ to 4, and the matrix elements interested in are eliminated (those of the form $\tilde{q}^*_p 2h\omega \cdot \tilde{q}^*_p 2h\omega$) Note that there is no cheating here: we could have done the same thing in the two shell case by keeping only the cross shell elements if we had wanted only the $\tilde{q}_p \cdot \tilde{q}_{p+1}$ component. To compare with empirical results in the $sd$, $p = 2$ shell we work at $h\omega = 11$. The standard one shell calculation yields $c^{20} = -2.40$ MeV (note that eq.\([13]\) gives $-2.37$ MeV). For the cross terms the large matrix produced

$$k = -2.80 \text{ MeV}, \quad <\tilde{q}^*_2 \tilde{q}_2> = 0.97, \quad (3.5)$$

$$<\tilde{q}^*_p 2h\omega | q_{02} + q_{13} + q_{24} > / N_{2h\omega} = 0.83 \quad (3.6)$$

where $q_{pp'}$ are the $2\hbar\omega$ quadrupole operators that can couple to $q_2$. Their sum is normalized to $N_{2h\omega}$. By normalizing each $q_{pp'}$ operator separately the overlap at 0.87 is slightly better, but it is the number in \([13]\) we shall need.

From \([3.3]\) $\tilde{q}^*_2 \approx \tilde{q}_2$, and this is an important message: it does not matter much to what $\tilde{q}_2$ is coupled - even $4\hbar\omega$ jumps if $H$ demands them (not very likely) - but it must be $\tilde{q}_2$ to ensure that “quadrupole renormalizes quadrupole” and that effective charges are state independent as shown below.

Proceeding as in eqs.\([3.1]\), we have (hc stands for Hermitian conjugate of the first term)

$$<i|H^\dagger_i|v'j' >= e_{20}(\omega) <i|\tilde{q}_p \cdot \tilde{q}_p |v'j' > - (3.7a)$$

$$\frac{k^2(\omega)}{2\hbar\omega} <i|q^*_{2h\omega} \cdot \tilde{q}_p + hc|J > <J|q^*_{2h\omega} \cdot \tilde{q}_p + hc|i'j' > = (3.7b)$$

$$\approx <i|e_{20}(\omega)\tilde{q}_p \cdot \tilde{q}_p - \frac{2k^2(\omega)}{\hbar\omega} \frac{1}{5}\tilde{q}^*_{2h\omega} \cdot q^*_{2h\omega} \tilde{q}_p \cdot \tilde{q}_p |i'j' > = (3.7c)$$

$$= (e_{20}(\omega) - \frac{k^2(\omega)}{\hbar\omega}) <i|\tilde{q}_p \cdot \tilde{q}_p |i'j' > = \frac{k^2(\omega)}{\hbar\omega} <i|q_p |v'j' > = <i|q_p |v'j' > - \frac{2k^2(\omega)}{2\hbar\omega} <i|q_{2h\omega}(q^*_{2h\omega} \cdot \tilde{q}_p + hc)|i'j' > = (3.8a)$$

$$<i|q_p |v'j' > - \frac{2k(\omega)}{\hbar\omega} \frac{1}{5}\frac{N_{2h\omega}}{N_p} <i|q_p \tilde{q}^*_{2h\omega} \cdot q^*_{2h\omega} |i'j' > = \frac{1}{5}\frac{N_{2h\omega}}{N_p} <i|q_p |i'j' > = (3.8b)$$

In the last step only half of the operators act: those creating first an excitation and then destroying it. Hence the factor 5/2 instead of 5. We have indulged in the fallacious approximation of treating the three terms in $q^*_{2h\omega} \equiv q^*_{2h\omega} - 2q_{p-2} + q^*_{2h\omega} + q_{p+2}$ as commuting with $\tilde{q}_p$, which is true only for the middle one. A correct calculation would yield a rank $2 + 3$ force for the offending terms. Still the result is correct for the two body contribution as can be checked in \([12]\) in which a very similar case is fully worked out. The neglect of three body contributions is common, but bad, practice.

The modification of the transition operator $q_p$ (not $\tilde{q}_p$) is calculated along similar lines,

$$<i|q_i |v'j' > = <i|q_p |v'j' > - \frac{2k^2(\omega)}{2\hbar\omega} <i|q_{2h\omega}(q^*_{2h\omega} \cdot \tilde{q}_p + hc)|i'j' > = (3.8a)$$

$$= \frac{1}{5}\frac{N_{2h\omega}}{N_p} <i|q_p \tilde{q}^*_{2h\omega} \cdot q^*_{2h\omega} |i'j' > = (3.8b)$$

$$= (1 - 0.83 \frac{k^2(\omega)}{\hbar\omega} \frac{N_{2h\omega}}{N_p}) <i|q_p |i'j' > = (3.8c)$$
What has been done is:

a) use the second order expression.

b) upon recoupling collect 4 equal terms and the factor 1/5. Then, to contract the normalized $2\hbar\omega$ operators (whose overlap is 0.83), interchange normalizations for $q_p$ and $q_{2\hbar\omega}$, and write

c) the final result.

Inserting the necessary numbers ($N_{2\hbar\omega}/N_p = 1.97$ for $p = 2$), the transition operator is boosted by a factor $(1+0.42)$, which is too small to agree with the empirical value close to 2. The problem is that second order perturbation may work very well for the energy but poorly for the transition rates [12]. We shall not go into the reasons, and simply borrow a nice argument due to Mottelson (15). The idea is that the second order perturbation should not be understood as affecting only the valence particles but the whole system. Then, calling $Q^{20}$ the total quadrupole operator, the estimate $Q^{20} = (1 + 0.42) q^{20}$ becomes

$$Q^{20} = q^{20} + 0.42 Q^{20} \longrightarrow Q^{20} = (1 - 0.42)^{-1} q^{20},$$

a result equivalent to an RPA resummation.

The comparison with empirical data is rewarding: ($\eta^\gamma$ are the effective charges)

$$e^{20} \longrightarrow e^{20}(1 + 0.3) = -3.12 \quad vs \quad 3.18 [16] \quad (3.9)$$

$$\eta^{20} = (1 - 0.42)^{-1} = 1.76 \quad vs \quad 1.78(3) [17] \quad (3.10)$$

$$\eta^{21} = (1 + 0.19)^{-1} = 0.8 \quad vs \quad 0.8(1) [14] \quad (3.11)$$

(The isovector effective charge can be calculated knowing $k=1.28$)

There is perhaps an element of luck here, but the presence of the overlap and the norms in the last equation (3.8) indicates that the diagonal representation is probably incorporating some important effects neglected in previous calculations of the effective charges [17].

The comparison of the effective pairing numbers in (3.2) with the empirical values would also be satisfactory, but fortuitous, because of the logarithmic divergence of second order theory. This problem does not seem to have attracted much attention, but there have been numerous controversies in the literature on the influence of core polarization in the strict sense - i.e. what we call multipole processes - on pairing renormalization (see [14] for a recent review).

According to our simple ideas “pairing renormalizes pairing” and “multipole renormalizes multipole” and the controversies would seem without object, but there is a catch.

A pairing force can always be written in the multipole representation, the highest multipoles entering with greater weights. In the $sd$ shell - the region that generated the controversies -, quadrupole and hexadecapole are already high multipolarities, well represented in the pairing decomposition, and their strong polarizabilities will have a non negligible effect. This is simply a manifestation of the lack of linear independence we have often encountered.

In heavier nuclei the important contributions to $H_C$ will become increasingly linear independent, and they will increasingly renormalize themselves, and the question will remain: what is the precise nature of pairing renormalization?

Whatever the answer to the question, it is clear that the use of diagonal representations simplifies considerably the calculation of effective operators by making it possible to concentrate attention on the few important terms that grow bigger, and neglect the small ones that have no chance to grow.

**IV. COMPARING INTERACTIONS**

Now we compare several realistic interactions in the $sd$ shell, the only region in which a direct fit to the data, $W$ [6], leads to more accurate spectra.

Table 4 shows some off diagonal matrix elements at the beginning of the shell, calculated with the KLS (as used in 2), KB [18], and Bonn B [19] realistic interactions, or taken from the $W$-fit. It is apparent that the realistic values are close to one another (especially KB and Bonn B) and not far from $W$, except in two cases.

The comparison of individual matrix elements can be misleading, because apparently large discrepancies may be of little consequence, and apparently small ones disastrous. Therefore it is better to concentrate on the contributions that can make a difference. Accordingly table 5 collects information on the lowest state in the $e$ and $E$ representations. The KB numbers have been left out because they practically duplicate those of Bonn B. The differences in eigenvalues between KLS and Bonn B is not large but may have some significance, while the agreement in eigenvectors is complete.
Very much the same is true in the comparison of \( W \) with the realistic values except for \( \Gamma = 20 \) and 30, which are not among the dominant states of the collective Hamiltonian. The reading of the result is simple: \( W \) has discovered and dealt with some local problem by altering radically some special matrix elements, but it has scrupulously respected the truly important contributions.

The local problem has several manifestations. In \(^{22}\text{Na}\) the realistic interactions produce a close doublet \( J = 1, 3 \), instead of the well detached \( J = 3 \) observed ground state [3], the \( \gamma \) band in \(^{24}\text{Mg}\) is too low, and more interesting for our purpose, the \( JT = 20 \) state in \(^{18}\text{F}\) always too low by about 1 MeV. (It should be noted that the experimental counterpart of this level is the second \( JT = 20 \) in \(^{18}\text{F}\), the first is an intruder).

The solution proposed by the \( W \) fit is such that there is no hope to reconcile it with the realistic forces. The problem is then to reconcile the latter with the data. We do not know how to do that, and we close this section by looking for some clues.

Though realistic interactions are similar, they also differ in some respects as can be gathered from fig. 3 of ref. [19], that shows different calculated spectra of \(^{18}\text{F}\) and \(^{18}\text{O}\). There are two effects.

- Overall Dilation. If we refer to eq. (1.8) the discrepancy can be absorbed by simply changing slightly the oscillator frequency, which is in principle fixed by the size of the nucleus. Because of their bad saturation properties this choice is not always possible for the realistic potentials. As long as saturation properties have to be treated phenomenologically, the overall dilation must be treated as a free parameter.

- The \( JT = 01 \) and 10 matrix elements. The differences due to overall dilation can be eliminated by normalizing the interactions to the same \( \sigma^2 \) in eq. (2.1). When this is done the most notable discrepancies come from the \( JT = 01 \) and 10 matrix elements, that are spectroscopically the lightest in the sense that \([JT]\) is smallest. As we have seen in the preceding section they are also the ones most severely affected by renormalization uncertainties.

Whether the local problem in the \( sd \) shell can be solved by playing on these different elements is an open question, but the analysis in terms of the diagonal representations makes clear that there is no much room for tampering with the dominant terms in the interactions.

**APPENDIX A:**

**Properties of the \( f \) matrices**

There is nothing special about the \( W \) matrix that is diagonalized in the \( E \) representation except that it is traceless by construction, while the \( f \) matrix leading to the \( e \) representation has a number of non trivial properties.

**Direct properties**

- The \( f^{\lambda T} \) matrix has twice as many elements as the \( W^{JT} \) matrix with \( J = \lambda \):

  if \( r \neq s \) and \( t \neq u \), \( W^{\lambda T}_{rstu} \) goes into \( \omega^{\gamma}_{rstu} \) and \( \omega^{\gamma}_{rust} \) and the allowed values of \( \Gamma \) and \( \gamma \) are the same.

  if \( r = s \) or \( t = u \), \( W^{\Gamma T}_{rstu} \) goes into \( \omega^{\gamma}_{rstu} = \omega^{\gamma}_{rust} \), but \( \Gamma \) is allowed for \((-)^{\Gamma} = -1 \) only and there is no restriction on \( \gamma \). E.g.: there are 5 possible ways of constructing \( J = 2 \) states in the \( sd \) shell \( d_{5/2}^2, d_{3/2}^2, d_{5/2}s_{1/2}, d_{5/2}d_{3/2}, s_{1/2}d_{3/2} \) and there are five \( JT = 21 \) states and three \( JT = 20 \) states (the first two are Pauli forbidden). For the \( \gamma \) matrices there are 8 possible combinations: the 5 above plus \( s_{1/2}d_{5/2}, d_{3/2}d_{5/2} \) and \( d_{3/2}s_{1/2} \) which are counted as different. Therefore in \( W \) we have a \( 3 \times 3 \) (\( \Gamma = 20 \)) and a \( 5 \times 5 \) (\( \Gamma = 21 \)) matrix; while in \( f \) we have twice an \( 8 \times 8 \) matrix. Each of these \( 8 \times 8 \) matrices consists of two blocks of \( 3 \times 3 \) and \( 5 \times 5 \) because of the following property.

- In the \( e \) representation we can write

\[
H = \frac{1}{2} \sum_{\gamma} [\gamma]^{1/2} \left[ (f^{\gamma}_{rstu} + (-)^{s-u} f^{\gamma}_{rtusu})(S^{\gamma}_{rstu} S^{\gamma}_{stu})^0 + (f^{\gamma}_{rstu} - (-)^{s-u} f^{\gamma}_{rtusu})(A^{\gamma}_{rstu} A^{\gamma}_{stu})^0 \right]
\]

(A1)

in terms of the \( S \) and \( A \) operators defined in eq. (1.31) of [1]. In the preceding example it means that out of 8 possible \( \gamma = 2\tau \) combinations 3 are of \( A \) type and 5 of \( S \) type. Note that the matrices are always symmetric but the eigenvectors are linear combinations of states that are either of \( S \) or \( A \) type.
• The trace of the $f$ matrix always vanishes, as seen from

$$
\sum_{\gamma,rt} f^2_{\gamma rt} = \sum_{rt} P_{rt} P_{tt} \sum_{\gamma \Gamma} (-)^{r+t-\gamma-\Gamma} \left\{ \begin{array}{ccc} r & r & \Gamma \\ t & t & \gamma \end{array} \right\} W^T_{rrtt} = \sum_{rt} P_{rt} P_{tt} W^0_{rrtt} = 0
$$

(A2)

where we have used (1.1c) and sum rule (A.19) from [1]. The matrix element $W^0_{rrtt}$ is always zero because it violates Pauli.

• The variance of the $f$ matrix is $\sigma^2_f = \frac{D-1}{8D} \sigma^2_W$, where $\sigma^2_W$ is the variance of the $W$ matrix. The calculation is better conducted in the $m$-scheme

$$
H(W) = \sum_{x} W_{xx'} Z_x^+ Z_{x'}
$$

$x \equiv (ij), x = 1 \ldots D^{(2)}/2, \ i < j \quad (A3)$

$$
H(f) = \sum_{a} f_{aa'} S_a S_{a'}
$$

$a \equiv (ij), x = 1 \ldots D^2 (ij \text{ unrestricted}) \quad (A4)$

A typical $W_{xx'} = W_{1234}$, say, appears as $f_{aa'} = \pm \frac{1}{4} W_{xx'}$ in four contributions: $aa' = 13 24$ and $24 13, 14 23$ and $23 14$. Then

$$
\sigma^2_W = \left( \frac{D^{(2)}}{2} \right)^{-1} \sum_{x} W^2_{xx'}
$$

$$
\sigma^2_f = D^{-2} \sum_{aa'} f^2_{aa'} = D^{-2} \sum_{a} \sum_{x} f^2_{aa'} = \frac{D-1}{8D} \sigma^2_W
$$

(A5)

(A6)

Asymmetric factorizations

Quadrupole renormalizations are mediated by terms of the form $k(\bar{q}_{p} \cdot \bar{q}_{2hw} + \bar{q}_{2hw} \cdot \bar{q}_{p})$. To understand how asymmetric factorization are possible we study the spectra of $I \times I$ matrices $f(n)$, whose non zero elements belong to the rectangular blocks $f_{xa}$ and $f_{ax}$, $a = 1 \ldots K, x = K + 1 \ldots I, I - K = L$.

Specializing eq.(1.2b) to this situation we have

$$
\sum_{x} f_{ax} u_{xk} = u_{ak} e_k \quad \sum_{a} f_{ax} u_{ak} = u_{zk} e_k
$$

(A7)

The eigenvector $|k\rangle$ with eigenvalue $e_k$ can be expanded in terms of unit column vectors $|i\rangle$ (1 in the $i$-th position, zero in the others):

$$
|k\rangle = \sum_{i=1,I} u_{ik} |i\rangle = \sum_{a=1,K} u_{ak} |a\rangle + \sum_{x=K+1,I} u_{zk} |x\rangle
$$

(A8)

By reversing simultaneously the sign of $e_k$ and $u_{zk}$ ($e_k \rightarrow -e_k, u_{zk} \rightarrow -u_{zk}, \forall x)$ eq.(A7) remains unchanged telling us that

$$
\bar{|k\rangle} = \sum_{a} u_{ak} |a\rangle - \sum_{x} u_{zk} |x\rangle
$$

(A9)

is an eigenvector with eigenvalue $-e_k$. Furthermore, from unitarity

$$
\sum_{i} u_{ik} u_{ik'} = \sum_{a} u_{ak} u_{ak'} + \sum_{x} u_{zk} u_{zk'} = \delta_{kk'}
$$

(A10)

and taking overlaps
\[ \langle k|k' \rangle = \sum_{a} u_{ak} u_{ak'} - \sum_{x} u_{xk} u_{xk'} = 0 \]  
(A11)

leading to

\[ \sum_{a} u_{ak} u_{ak'} = \sum_{x} u_{xk} u_{xk'} = \frac{1}{2} \delta_{kk'} \]  
(A12)

From these results we may construct the spectrum of \( f(n) \). Let’s call \( M = \min(L, K) \). We have: \( M \) positive eigenvalues \( e_k \) \( (k = 1, M) \), \( M \) negative ones \( \bar{e}_k = -e_k \) \( (k = M + 1) \) and \( I - 2M \) null ones.

We may gain further insight by presenting the problem as a search for an optimum approximant \( g_a g_x \) to the rectangular matrix \( f_{ax} \), defined through

\[ \sum (f_{xa} - g_a g_x)^2 = \min \]  
(A13)

Variation with respect to \( f_x \) and \( f_a \) leads to

\[ \sum_x f_{xa} g_x = g_a \sum_x f_x^2, \quad \sum_a f_{xa} g_a = g_x \sum_a g_a^2 \]  
(A14)

and given that \((\ref{A13})\) is invariant under \( g_x \rightarrow \sigma g_x \) \( g_a \rightarrow \sigma^{-1} g_a \) we may request

\[ \sum_x g_x^2 = \sum_a g_a^2 = e \]  
(A15)

and \((\ref{A14})\) becomes \( (\ref{A7}) \) by identifying \( g_x = u_{xk} \), \( g_a = u_{ak} \), \( e = e_k \). The factorization produced by the lowest \((k = 1)\) eigenstate at \( e = -|e_1| \) is identical to the one for the highest at \( e = |e_1| \) and the best available. Exact separability is achieved for \( e_k = 0 \) for \( k \neq 1 \).

**APPENDIX B:**

**Baranger and Kumar revisited.**

In two famous papers Baranger and Kumar attempted to derive from a realistic interaction the pairing plus quadrupole forces adapted to a space of two major shells [20] and proceeded to do Hartee-Fock-Bogoliubov (HFB) calculations in the rare earth region that showed for the first time that it was possible to explain microscopically the onset of deformation [21].

The success of the calculations is probably due in large part to the fact that the model is far more realistic than its authors believed. The reason is rather strange and we think it is worth telling.

Let us start by comparing the traditional pairing plus quadrupole forces as used in [21,21]

\[ H_P = -G_x (P^+_p + P^+_p) \cdot (P_p + P_{p+1}) \]  
(B1)

\[ H_q = -\frac{\chi'}{2} (q_p + q_{p+1}) \cdot (q_p + q_{p+1}) \]  
(B2)

with the normalized versions in eqs. (1.9) and (1.10), which we write explicitly by borrowing numbers from table II and remembering that \( \hbar \omega_0 = 9 \text{ MeV} \):

\[ H_P = -0.32 \hbar \omega \left( \frac{P^+_p}{\sqrt{\Omega_p}} + \frac{P^+_p}{\sqrt{\Omega_{p+1}}} \right) \cdot \left( \frac{P_p}{\sqrt{\Omega_p}} + \frac{P_{p+1}}{\sqrt{\Omega_{p+1}}} \right) \]  
(B3)

\[ H_q = -0.216 \hbar \omega \left( \frac{q_p}{N_p} + \frac{q_{p+1}}{N_{p+1}} \right) \cdot \left( \frac{q_p}{N_p} + \frac{q_{p+1}}{N_{p+1}} \right). \]  
(B4)

If we consider first the case of one shell, the operators are the same, and we can relate the coupling constants by simply equating.

For the two shell case, the overlap
interaction (see Note 2 at the end of the section). Then they proceeded to invent another method to obtain the coupling constant, unrelated to any extraction which - though in a primitive form - is identical to ours and correct to within some details (discussed when faced with this unwanted reduction, instead of blaming the \( p \) for one shell, reduced by a factor of about 0.6 for two shells at midshell situation, as in \(^{28}\)Si, the \( p + 1 \) - upper - shell is very poorly represented in the wavefunctions. Then the large overlap is meaningless.

With this proviso in mind we equate the traditional and the new forms. Recalling that \( \hbar \omega = 40 A^{-1/3} \) \(^{22}\), and writing the norms in terms of \( A_{mp} \) as in eqs.(6,7) we find for one shell

$$\frac{0.216 \hbar \omega}{N_p^2} \equiv \frac{1}{2} \frac{216}{A^{1/3} A_{mp}^{4/3}} = \frac{\chi}{2} = \frac{\chi_0}{2} A^{-5/3}; \quad \frac{0.32 \hbar \omega}{\Omega_p} \equiv \frac{19.51}{A^{1/3} A_{mp}^{2/3}} = G \equiv G_0 A^{-2/3}$$

(B7)

and for two shells,

$$\frac{0.216(2 \hbar \omega)}{N_p^2 + N_{p+1}^2} \equiv \frac{1}{2} \frac{216}{A^{1/3} A_{mp}^{4/3}} = \frac{\chi}{2} = \frac{\chi_0}{2} A^{-5/3}; \quad \frac{0.32(2 \hbar \omega)}{\Omega_p + \Omega_{p+1}} \equiv \frac{19.51}{A^{1/3} A_{mp}^{2/3}} = G \equiv G_0 A^{-2/3}$$

(B8)

where we have expressed the averaged norms in terms of \( A_{mp} \) and \( A_{c'p} \), both close enough to the total number of particles at the closure of shell \( p \), \( A_{cp} \), to be identified with it in what follows.

For one shell the only problem comes from the conventional scalings, in \( A^{-5/3} \) and \( A^{-2/3} \). It is possible to understand their origin: they amount to set \( A_{mp} = A \), which makes sense in comparing strengths in distant regions, but is locally wrong. If taken at face value, the \( A^{-5/3} \) local behaviour predicts variations in the moments of inertia of neighbouring that are much larger than the observed ones \(^{23,24}\).

In the two shell case the couplings are reduced with respect to the one shell values by a factor of about

$$\left( \frac{A_{mp}}{A_{cp}} \right)^{k/3} = \left( \frac{2p + 3}{2p + 4} \right)^k,$$

where \( k = 4 \) for \( \chi \) and \( k = 2 \) for \( G \). If our identifications where correct these discrepancies should not exist, and they are related to the risk we described after eq. (B6). There is no guarantee that we can approximate well the operator \( q_p + q_{p+1} \) by \( q_p + q_{p+1} \). The compromise \( \chi \) in (B8) is too small for the lower shell but also too large for the upper one. If the mixing is strong and both shells contribute equally to the wavefunctions, then the large overlap in (B6) indicates that the compromise may work but in a nucleus well described by the lower shell alone it makes no sense. The thing to do in this case is to restrict the model to one shell.

By overlapping the \( q \cdot q \) form with a realistic interaction Baranger and Kumar had obtained \( \chi_0 = 203 \) vs our 216 for one shell, reduced by a factor of about 0.6 for two shells at \( p = 2 \), close to the value of 7/8 calculated in eq. (B3). When faced with this unwanted reduction, instead of blaming the \( q \cdot q \) form, they declared incorrect their method of extraction which - though in a primitive form - is identical to ours and correct to within some details (discussed in section II). Then they proceeded to invent another method to obtain the coupling constant, unrelated to any interaction (see Note 2 at the end of the section).

At this point ref. \(^{20}\) becomes confusing because it is argued that since the quadrupole force cannot be extracted from the realistic interaction its origin must be something else that may not be quadrupole at all. What we are showing is that the “something else” is simply the normalized quadrupole force.

The extraordinary thing is that Baranger and Kumar had found it! The reason they did not see what they had found is that they reasoned in terms of the \( A^{-5/3} \) scaling, in spite of having given the correct argument about what the scaling must be!

Now observe carefully eqs.(B7) and (B8) to discover the miracle that repairs the damage. The only sensible way to define \( \chi_0 \) for one shell is to “equate” \( A_{mp} \approx A \), while for two shells we must take \( A_{cp} \approx A \) and now \( \chi_0 \) is identical to 216 in both cases!

There is no contradiction between

\( \chi'(1 \text{shell}) \neq \chi'(2 \text{shells}) \) at a given nucleus and
\( \chi_0'(1 \text{shell}) = \chi_0'(2 \text{shells}), \) both calculated in different nuclei.

This is the subtle argument missing in \(^{20}\). It is only thanks to universal scaling that it can be made.

Everything seems to happen as if one flaw of the model - incorrect scaling - corrected the other: the space dependence of the coupling constants. A better interpretation though, is that the model should be restricted either to one shell in the vicinity of \( A_{mp} \), or to two shells in the vicinity of \( A_{cp} \).
Now we note that the rare earth region studied in [21] is approximately centered at the oscillator closures $Z=70$ and $N=112$, which meets this restriction, and that the parameters used were (in Mev):

$$\chi' \approx 280, \quad G_{0\pi} = 27 \quad G_{0\nu} = 22,$$

somewhat larger than those in eq.(B8) but quite consistent with the renormalized values of section III. (The need to use different $G_0$ values for neutrons and protons is readily explained by [B8]. It is a mild manifestation of space dependence).

We can draw two conclusions:

i) the conventional pairing plus quadrupole model in two shells is far more consistent with the realistic interactions than its authors believed.

ii) it can be made truly realistic by using the normalized operators, by including a pair of other terms (octupole and hexadecapole), and by examining more closely the monopole contribution. Very little of the basic simplicity of the original will be lost in this improved version.

**Note 1. On space dependence.**

Examine what happens in larger spaces when eq.(B8) is generalized to $M$ major shells. It is elementary to prove that $\chi' = O(A^{-1/3}M^{-4})$, and the overlap tends to $\sqrt{5/9}$ and $\chi' = O(A^{-1/3}M^{-4})$. It means that to simulate - never mind how remotely - the behaviour of its realistic counterpart, the conventional $q \cdot q$ force must be affected by a vanishingly small $\chi'$.

**Note 2. On the second method of extraction in [20].** To replace direct extraction of $\chi'$ from the realistic interaction Baranger and Kumar proposed a method based on the idea that the average energy of a nucleus is independent of its shape. It makes no reference to the force nor to any empirical datum. It leads to:

$$\chi' = \frac{\hbar \omega}{N_p^2 + N_{p+1}^2}$$

( eqs.(72,73) and paragraph following them in [20], but here we have introduced the norms instead of their asymptotic values). This is the same $\chi'$ of eq.(B8), except that a factor $4 \times 0.216$ has been set to unity. The identity in form suggests that the method is a valid dimensional analysis, but the similarity in the numbers is likely to be accidental.

**TABLE IV.** Comparison of some matrix elements in the $sd$ shell ($5 = d_{5/2}$, $3 = d_{3/2}$, $1 = s_{1/2}$) for different interactions. $\leftarrow$ indicates large W-realistic discrepancies.

| rstu JT | KLS | KB | Bonn B | W |
|---------|-----|----|--------|----|
| 5553    | 10  | 3.03 | 3.17 | 3.31 | 2.54 |
|         | 21  | -0.52 | -0.40 | -0.22 | -0.28 |
|         | 30  | 1.21 | 1.87 | 1.89 | 2.22 |
|         | 41  | -1.24 | -1.36 | -1.28 | -1.24 |
| 5533    | 01  | -4.17 | -3.79 | -3.41 | -3.19 |
|         | 10  | 1.45 | 1.62 | 1.29 | 0.72 |
|         | 21  | -0.89 | -0.90 | -0.89 | -1.62 |
|         | 30  | 0.13 | 0.50 | 0.56 | 1.89 $\leftarrow$ |
| 5153    | 20  | -1.10 | -1.44 | -1.33 | -0.1 $\leftarrow$ |

**TABLE V.** Lowest energies $E_\Gamma$ for $\Gamma = 01, 10, 20$ and 30 and $e^\gamma$ for all $\gamma$, and overlaps of the wavefunctions for KLS, Bonn B and W.

| $01$ | $10$ | $20$ | $30$ | $e^0$ | $e^1$ | $e^2$ | $e^3$ | $e^4$ | $<KLS|Bonn B>$ | $<KLS|W>$ |
|------|------|------|------|-------|-------|-------|-------|-------|----------------|----------|
| -5.42 | -5.43 | -5.68 | -5.15 | KLS | -2.18 | 2.38 | -2.90 | -0.71 | -0.82 | 0.44 | -1.61 | 0.40 |
| -5.42 | -6.24 | -5.91 | -2.66 | Bonn B | -1.55 | 2.64 | -3.32 | -0.97 | -0.83 | 0.46 | -1.39 | 0.52 |
| -5.69 | -5.90 | -2.95 | -2.44 | W | -2.16 | 3.08 | -3.18 | -0.70 | -0.94 | 0.54 | -1.60 | 0.51 |
| 1.00 | 1.00 | 1.00 | 1.00 | $<KLS|Bonn B>$ | 0.99 | 1.00 | 1.00 | 0.99 | 0.98 | 1.00 | 1.00 |
| 1.00 | 0.98 | 0.55 | 0.82 | $<KLS|W>$ | 0.95 | 0.99 | 1.00 | 0.98 | 0.92 | 1.00 | 1.00 |
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FIG. 1. $E$-eigenvalue density for the KLS interaction in the pf+sdg major shells $\hbar \omega = 9$. Each eigenvalue has multiplicity [Γ]. The largest ones are shown by arrows.

FIG. 2. $e$-eigenvalue density for the KLS interaction in the pf+sdg major shells. Each eigenvalue has multiplicity [γ]. The largest ones are shown by arrows.
FIG. 3. $E$-eigenvalue density for the KLS interaction in the pf+sdg major shells $\hbar\omega = 9$, after removal of the five largest multipole contributions. Each eigenvalue has multiplicity $\Gamma$. The largest ones are shown by arrows.

FIG. 4. $E$-eigenvalue density for the KLS interaction in the pf+sdg major shells $\hbar\omega = 9$, after removal of multipole contributions with $|\epsilon| > 1.3$. Each eigenvalue has multiplicity $\Gamma$. The largest ones are shown by arrows.