Realistic collective nuclear Hamiltonian

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(Received 13 April 1995; revised manuscript received 24 April 1996)

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 retain the simplicity of the traditional pairing plus multipole models, while eliminating their flaws through a normalization mechanism dictated by a universal $A^{-1/3}$ scaling. Coupling strengths and effective charges are calculated and shown to agree with empirical values. Comparisons between different realistic interactions confirm the claim that they are very similar. [S0556-2813(96)05610-5]

PACS number(s): 21.60.Cs, 21.60.Ev, 21.30.−x

I. INTRODUCTION

It has not been possible, yet, to construct interactions that could satisfy simultaneously three basic conditions: (A) to be realistic, i.e., consistent with the nucleon-nucleon (NN) phase shifts, (B) to ensure good saturation properties, i.e., correct binding energies at the observed radii, and (C) to provide good spectroscopy. As a consequence many forces have been designed for specific contexts or problems: pairing plus quadrupole [1,2], density-dependent potentials for mean-field approaches [3,4], Landau-Migdal parametrizations for studies of the giant resonances [5], direct fits to two-body matrix elements for shell-model calculations [6], and many others. A way out of this unsatisfactory state of affairs would be to exhibit an interaction consistent with conditions (A)–(C) above. To understand how the project can be implemented, let us start by assuming that we work in a Fock representation. Then the Hamiltonian $\mathcal{H}$ is given in terms of a set of matrix elements which we take to be written in an oscillator basis, the natural one for self-bound systems.

It may be thought very uneconomic to use an infinite set of numbers to characterize $\mathcal{H}$, but there is a great advantage in doing so, because it becomes possible to prove the following separation property.

Given a sufficiently smooth Hamiltonian $\mathcal{H}$, it can be separated as $\mathcal{H}=\mathcal{H}_m+\mathcal{H}_M$. Only the monopole field $\mathcal{H}_m$ is affected by spherical Hartree-Fock variation. Therefore it is entirely responsible for global saturation properties and single-particle behavior.

The idea is that $\mathcal{H}$ can be written in terms of density operators coupled to good angular momentum λ [i.e., $(a^\dagger a)^\lambda$], and that $\mathcal{H}_m$ exhausts the contributions with $\lambda=0$, while the multipole part $\mathcal{H}_M$ contains all the rest. A schematic proof of the separation property has been given in [7], and a more complete one may be found in [8]. It is easy to explain the interest in this result.

One of the major problems of nuclear physics is that realistic forces have bad saturation properties and since $\mathcal{H}_m$ is in charge of them it must be treated phenomenologically. Fortunately, it is a relatively simple object that makes it quite feasible to force good saturation in a shell-model context, with the pleasing result that the multipole part $\mathcal{H}_M$, which can be extracted rather uniquely from the realistic interactions, has an excellent behavior [9,10]. Therefore conditions (A) and (C), as well as (B) and (C), are mutually compatible.

An elementary argument explains the situation. The observed nuclear radii $r\cong 1.2A^{1/3}$ fm imply average interparticle distances of some 2.4 fm, and therefore the nucleons ''see'' predominantly the medium range of the potential. This is a region that is well understood theoretically [11] and well described by the realistic forces.

The saturation problem remains, of course, and as long as conditions (A) and (B) cannot be made compatible, a phenomenological treatment of $\mathcal{H}_m$ will be necessary. Some progress has been already made in this respect: In Ref. [12], a hint that will emerge in the present paper has been taken up and applied to the construction of a mass formula that is extremely precise by present standards (rms error of 375 keV for all known nuclei with $N,Z>8$). Of the 28 parameters that enter the calculations, a dozen represent a first approximation to the monopole field. It is still very crude but it makes plausible the idea of constructing some simple $\mathcal{H}_m$ that contains few parameters and describes nuclear data satisfactorily. Since something simple in Fock space may be complicated in coordinate space, it may point to ways—so far overlooked—of reconciling conditions (A) and (B).

It follows that, although we still fall short of a complete and rigorous characterization of $\mathcal{H}$, we may not be far from it. In particular, we know $\mathcal{H}_M$ well. As this knowledge comes in huge arrays of matrix elements, it would be more helpful if we could extract from this mass of numbers the truly important ones, i.e., separate $\mathcal{H}_M=\mathcal{H}_C+\mathcal{H}_R$, into a collective ($C$) part and a rest that could be treated as random (R). There are many advantages in doing so, but one is special. As new regions open to scrutiny, through Monte Carlo techniques [13] and further improvements in shell model technology [14], the nature of the problems changes: Dimensionalities grow exponentially with the size of the systems, but the behavior described by the enormous matrices also becomes simpler through the increasing influence of coherent effects.

The special advantage is that in adapting existing methods to face this situation, or designing new ones, our basic tool is the Hamiltonian itself, and the simpler it can be made, the higher will be the chances of developing successful computational strategies.

Clearly, a deeper understanding of $\mathcal{H}_M$ is called for.

In Sec. II 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 Sec. III, the possible candidates to $\mathcal{H}_C$ are examined, and then it is explained how a given choice of dominant terms is optimally extracted from the Hamiltonian, ensuring that the corresponding coupling constants are quantitatively correct.

Section IV proposes an analytic calculation of second order renormalizations due to core polarization effects. The agreement with empirical values turns out to be excellent.

Section V is devoted to a comparison of different realistic interactions among themselves—which establishes their unicity—and with the W fit in the sd shell [6].

Appendix A contains a brief summary of the elementary angular momentum results that are needed. With few exceptions the material is borrowed or adapted from Refs. [15,16], and the aim of this appendix is to make the whole presentation self-contained.

Appendix B is devoted to some results on the matrix defining the diagonal multipole representation.

Appendix C revisits the pairing plus quadrupole model.

II. DIAGONAL REPRESENTATIONS OF $\mathcal{H}$

Our plan is as follows: (a) Introduce $\mathcal{H}_M$ 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 (e) say a few words about the consequences of this result on the specification of $\mathcal{H}_m$.

A. Hamiltonian

We start by calling upon Eqs. (A20)–(A23) to write $\mathcal{H}_M$ in the normal and multipole representations:

$$\mathcal{H}_M=\sum_{r\leqslant s,t\leqslant u,\Gamma} W^{\Gamma}_{rstu}Z^{\dagger}_{rs\Gamma}\cdot Z_{tu\Gamma}\,, \tag{2.1a}$$

$$\mathcal{H}_M=\sum_{rstu\Gamma}[\gamma]^{1/2}\frac{(1+\delta_{rs})^{1/2}(1+\delta_{tu})^{1/2}}{4}\omega^{\gamma}_{rtsu}(S^{\gamma}_{rt}S^{\gamma}_{su})^0, \tag{2.1b}$$

$$\omega^{\gamma}_{rtsu}=\sum_{\Gamma}(-)^{s+t-\gamma-\Gamma}\begin{Bmatrix} r & s & \Gamma\\ u & t & \gamma\end{Bmatrix}W^{\Gamma}_{rstu}[\Gamma], \tag{2.1c}$$

$$W^{\Gamma}_{rstu}=\sum_{\gamma}(-)^{s+t-\gamma-\Gamma}\begin{Bmatrix} r & s & \Gamma\\ u & t & \gamma\end{Bmatrix}\omega^{\gamma}_{rtsu}[\gamma]. \tag{2.1d}$$

We use W for the matrix elements to stress that the interaction has been made monopole free. Since $\mathcal{H}_m$ is defined as containing all the $\gamma=00$ and 01 terms, $\mathcal{H}_M$ is defined by

$$\omega^{\gamma}_{rstu}=0 \quad \text{for} \quad \gamma=00 \quad \text{and} \quad 01.$$

The one-body contractions vanish identically for $\mathcal{H}_M$ because they are proportional to $\omega^{0\tau}_{rstu}$.

The normal form is unique and the ordering of the indices simply eliminates double counting: The contributions in $rstu$, $srtu$, $rsut$, and $srut$ are identical, and it is just as well to keep only the first.

The multipole form is highly nonunique because the terms are not linearly independent and permuting indices leads to different objects. We have chosen the variant in which summations are unrestricted for a reason that will become immediately apparent [after Eq. (2.3b)].

For the calculations we adopt the Kahana-Lee-Scott (KLS) force [17,18], but in Sec. V it is argued that the choice of *realistic* interaction does not matter much.

B. Separable form

We call H_M the restriction of $\mathcal{H}_M$ to a finite set of orbits. Replacing pairs by single indices $rs\equiv x$, $tu=y$ in Eq. (2.1a) and $rt\equiv a$, $su=b$ in Eq. (2.1b), we bring the matrices W^{Γ}_{xy} and $f^{\gamma}_{ab}=\omega^{\gamma}_{ab}\sqrt{(1+\delta_{rs})(1+\delta_{tu})}/4$ to diagonal form through unitary transformations $U^{\Gamma}_{xk},u^{\gamma}_{ak}$:

$$U^{-1}WU=E\Rightarrow W^{\Gamma}_{xy}=\sum_k U^{\Gamma}_{xk}U^{\Gamma}_{yk}E^{\Gamma}_k\,, \tag{2.2a}$$

$$u^{-1}fu=e\Rightarrow f^{\gamma}_{ab}=\sum_k u^{\gamma}_{ak}u^{\gamma}_{bk}e^{\gamma}_k\,, \tag{2.2b}$$

and, then,

$$H_M=\sum_{k,\Gamma}E^{\Gamma}_k\sum_x U^{\Gamma}_{xk}Z^{\dagger}_{x\Gamma}\sum_y U^{\Gamma}_{yk}Z_{y\Gamma}\,, \tag{2.3a}$$

$$H_M=\sum_{k,\gamma}e^{\gamma}_k\Big(\sum_a u^{\gamma}_{ak}S^{\gamma}_a\sum_b u^{\gamma}_{bk}S^{\gamma}_b\Big)^0[\gamma]^{1/2}, \tag{2.3b}$$

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

C. Dominant terms

We have calculated the eigensolutions in Eqs. (2.3a) and (2.3b) 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 B: 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 a few of them are neatly detached. The strongest have $\gamma^{\pi}=1^-0,\,1^+1,\;2^+0,\;3^-0$, in Eq. (2.3b) *and the associated H in* Eq. (2.3a) *is recalculated; the E distribution becomes quite symmetric*. Details will be given in Sec. III,

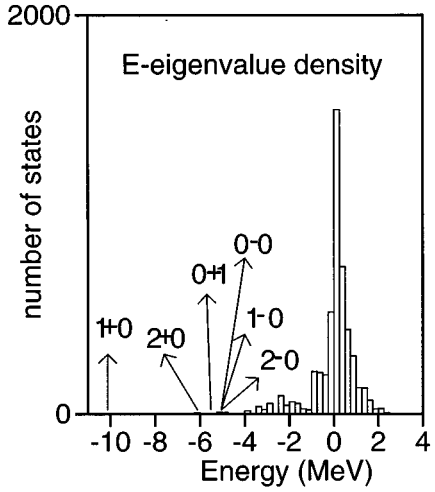

FIG. 1. E-eigenvalue density for the KLS interaction in the $pf+sdg$ major shells ($\hbar\omega=9$). Each eigenvalue has multiplicity [Γ]. The largest ones are shown by arrows.

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 MeV.

This result is most telling because from the work of Mon and French [19] 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 Γ peaks—the very few dominant terms in the e distribution are responsible for deviations from random behavior in H_M. Positively stated, these terms 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 will be analyzed, we include the $\Gamma=10$ and 01 terms, and the six strongest γ ones.

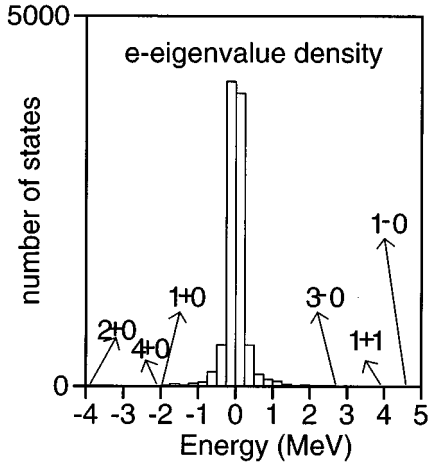

FIG. 2. e-eigenvalue density for the KLS interaction in the pf +sdg major shells. Each eigenvalue has multiplicity [γ]. The largest ones are shown by arrows.

Their eigenstates [i.e., the factors in Eqs. (2.3a) and (2.3b) 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:

$$\overline{P_p^\dagger}\equiv\overline{P_{01p}^\dagger}=\sum_{r\in p} Z_{rr01}^\dagger \Omega_r^{1/2}/\Omega_p^{1/2}, \quad \Omega_p\cong 0.655A_{mp}^{2/3}, \tag{2.4}$$

$$\overline{q_p}\equiv M_p^{20}=\sum_{rs\in p} S_{rs}^{20} q_{rs}/\mathcal{N}_p, \quad \mathcal{N}_p^2\cong 0.085A_{mp}^{4/3}, \tag{2.5}$$

where

(i) $\Omega_r=j_r+1/2$, $q_{rs}=\sqrt{\frac{1}{5}}\langle r\|r^2Y^2\|s\rangle$,

(ii) A_{mp} is the the total number of particles at midshell p [$p^{(2)}=p(p-1)$, remember],

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

(iii) the norms Ω_p and $\mathcal{N}_p$ are then

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

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

For the calculation of $\mathcal{N}_p^2$ we have used the matrix elements listed in Eq. (A34). Note that they should multiplied by a factor $\sqrt{2}$, since they are reduced with respect to j only, while q_{rs} is reduced with respect to spin and isospin.

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. Labeling the orbits by their l quantum numbers, we have two pairing terms

$$\overline{P_{ST}^\dagger}=\left(\sum_l [l]\right)^{-1/2}\sum_l [l]^{1/2}Z_{ll0ST}^\dagger, \quad ST=01,10,$$

which in jj coupling become

$$\overline{P_{01}^\dagger}=\Omega_p^{-1/2}\sum_r \sqrt{\Omega_r}Z_{rr01}^\dagger$$

and

$$\overline{P_{10}^\dagger}=\Omega_p^{-1/2}\sum_{j,j'}[l]^{1/2}\{(ll)0\,(1/2\,1/2)1\,|(jj')1\}Z_{rr'10}^\dagger, \tag{2.6}$$

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 P_{10} and P_{01}. The orbits are labelled by their j values.

rs	$\overline{P_{01}}$	$(U^{01}_{rs})_{3,4}$	$\sqrt{2}(U^{01}_{rs})_{3+4}$	$\overline{P_{10}}$	$(U^{10}_{rs})_{3,4}$	$\sqrt{2}(U^{10}_{rs})_{(3+4)}$
77	-0.63	-0.65	-0.66	0.41	0.31	0.31
75				-0.68	-0.74	-0.74
33	-0.45	-0.38	-0.41	0.33	0.26	0.27
35				0	-0.30	-0.25
31				-0.42	-0.43	-0.44
55	-0.55	-0.58	-0.59	-0.27	-0.12	-0.13
11	-0.32	-0.29	-0.31	-0.04	0.07	0.04
E^{Γ}_3		-2.95			-4.59	
99	0.58	0.61	0.64	-0.37	-0.26	-0.25
97				0.63	0.67	0.72
77	0.52	0.55	0.57	0.26	0.12	0.11
75				0	-0.27	-0.28
55	0.45	0.41	0.34	-0.31	-0.22	-0.20
53				0.46	0.50	0.48
33	0.37	0.35	0.28	0.16	0.03	0.01
31				0	-0.21	-0.18
11	0.26	0.17	0.13	-0.26	-0.22	-0.20
E^{Γ}_4		-2.65			-4.78	
$\frac{1}{2}E^{\Gamma}_{3+4}$			-2.76			-5.06

where we have recovered the usual $r\equiv jl$ 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 P_{p01} accounts very well for $(U^{01}_{rr})_p$. For P_{p10} vs $(U^{10}_{rs})_p$ the agrement is not so excellent, but still good. The overlaps are found under $\langle U_p|P\rangle$ in Table II, which also contains the corresponding values of $\langle u_p|M\rangle$ for the lowest multipole operators M. The agreement is again excellent except for the σ case, for which it is only fair. Note that the form of these operators is given in Appendix A.

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

$$U_{3+4}=(\alpha U'_3+\beta U'_4)/\sqrt{2},\quad \alpha^2+\beta^2=2, \tag{2.7}$$

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, both for the U_i and u_i vectors, as Table II shows: $\langle U_i|U'_i\rangle$ and $\langle u_i|u'_i\rangle$ are strikingly close to 1 with no exceptions while α^2 is quite close to 1.

Therefore, for any *normalized* pairing or multipole operator O we have the following.

If O_p and O_{p+1} are eigenvectors for shell p and $p+1$ separately, then (O_p+O_{p+1}) is very much the eigenvector 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 eigenvectors so as to halve its eigenvalue.

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) and they have identical structure.

The dominant negative parity contributions are $\gamma=10$ at 4.59 MeV, $\langle rY^1|u^{10}\rangle=0.994$ and $\gamma=30$ at 2.69 MeV, $\langle r^3Y^3|u^{30}\rangle=0.986$.

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 $(M^{\gamma}M^{\gamma})^0=(-)^{\gamma}[\gamma]^{-1/2}(M^{\gamma}\cdot M^{\gamma})$.]

D. Universal scaling

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We have now the necessary elements to construct a schematic but accurate collective Hamiltonian. From [9] we know that

$$W^{\Gamma}_{xy}(\omega)\cong\frac{\omega}{\omega_0}W^{\Gamma}_{xy}(\omega_0) \tag{2.8}$$

(ω is the oscillator frequency) and therefore the eigenvalues

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

γ	e^{γ}_3	e^{γ}_4	e^{γ}_{3+4}	M	$\langle u_3\|M\rangle$	$\langle u_4\|M\rangle$	$\langle u_3\|u'_3\rangle$	$\langle u_4\|u'_4\rangle$	α^2
11	1.77	2.01	3.90	$\sigma\tau$	0.992	0.994	0.999	1.000	0.94
20	-1.97	-2.14	-3.88	r^2Y_2	0.996	0.997	1.000	1.000	0.95
10	-1.02	-0.97	-1.96	σ	0.880	0.863	0.997	0.994	1.04
21	-0.75	-0.85	-1.60	$r^2Y_2\tau$	0.991	0.998	0.999	0.997	0.94
Γ	E^{Γ}_3	E^{Γ}_4	E^{Γ}_{3+4}	P	$\langle U_3\|P\rangle$	$\langle U_4\|P\rangle$	$\langle U_3\|U'_3\rangle$	$\langle U_4\|U'_4\rangle$	α^2
01	-2.95	-2.65	-5.51	P_{01}	0.992	0.998	1.000	0.994	1.048
10	-4.59	-4.78	-10.12	P_{10}	0.928	0.910	0.998	0.997	0.991

TABLE III. The $sdg+pf$ peaks in the f representation ($|e_\gamma|>1.3$) and their pf and sdg counterparts. $\mathcal{S}^\pi$, $\mathcal{A}^\pi$= symmetry type and parity. ⇑ signals the peaks singled out in Fig. 2, and their one-shell counterparts. ↓ is for peaks with $|e_\gamma|<1.3$ MeV that are likely to have a clear multipole character. Parentheses indicate that the assignment is unchecked but given as plausible.

$\lambda\,\tau$	Sym	Type	e_{pfsdg}		e_{pf}	e_{sdg}	
00	$\mathcal{A}^-$	...	1.88				
10	$\mathcal{S}^-$	r_1Y_1	4.59	⇑			
	$\mathcal{S}^\dagger$	σ	-1.96	⇑	-1.02	-0.97	⇑
	$\mathcal{S}^-$	...	-1.53				
	$\mathcal{S}^\dagger$	l	1.44		0.66	0.80	
	$\mathcal{S}^-$	...	1.41				
11	$\mathcal{S}^\dagger$	$\sigma\tau$	3.90	⇑	1.77	2.01	⇑
	$\mathcal{A}^-$	...	-1.83				
	$\mathcal{S}^-$	$r_1Y_1\tau$	1.81				
20	$\mathcal{S}^\dagger$	r^2Y_2	-3.88	⇑	-1.97	-2.14	⇑
	$\mathcal{S}^\dagger$	...	1.31		0.64	0.75	
21	$\mathcal{S}^\dagger$	$r^2Y_2\tau$	-1.60		-0.75	-0.85	
	$\mathcal{S}^-$	$M2??$	-1.55				
	$\mathcal{A}^\dagger$	...	1.46		0.64	0.76	
30	$\mathcal{S}^-$	r^3Y_3	2.69	⇑			
31	$\mathcal{S}^-$	$r^3Y_3\tau$	1.14	↓			
40	$\mathcal{S}^\dagger$	(r^4Y_4)	-2.11	⇑	-1.12	-1.24	⇑
41	$\mathcal{S}^\dagger$	$(r^4Y_4\tau)$	-0.91	↓			
50	$\mathcal{S}^-$	(r^5Y_5)	1.75				
51	$\mathcal{S}^-$	$(r^5Y_5\tau)$	0.78	↓			
60	$\mathcal{S}^\dagger$	(r^6Y_6)	-1.26	↓	-0.73	-0.82	

in Table II must scale in the same way. Setting $\alpha^2=1$ in Eq. (2.7) for simplicity, the *normalized* pairing and quadrupole forces become

$$H_{\overline{P}}=-\frac{\hbar\omega}{\hbar\omega_0}|E^{01}|(\overline{P^\dagger_p}+\overline{P^\dagger_{p+1}})\cdot(\overline{P_p}+\overline{P_{p+1}}),\qquad(2.9)$$

$$H_{\overline{q}}=-\frac{\hbar\omega}{\hbar\omega_0}|e^{20}|(\overline{q_p}+\overline{q_{p+1}})\cdot(\overline{q_p}+\overline{q_{p+1}}),\qquad(2.10)$$

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 $e_1^\gamma\cong e_2^\gamma\cong e_{1+2}^\gamma/2$ (same for E^Γ), 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*.

To give a full characterization of $\mathcal{H}_M$, Eqs. (2.9) and (2.10) should be generalized to any number of shells. For the quadrupole (and other multipole terms) this would demand inclusion of $\nu\hbar\omega$ excitations, and in Sec. IV, it will be shown that the $\gamma=2\tau$ operator q'_p that couples shell p to $2\hbar\omega$ jumps, remains indeed close to q_p, with welcome consequences. Here we concentrate on the restricted generalization of Eqs. (2.9) and (2.10) obtained by simply summing over all p values.

A formal proof would start from the remark that it is always possible to diagonalize in some sufficiently large space, and therefore write the lowest state associated with multipole γ as $\Sigma\mathcal{O}_p^\gamma/\mathcal{N}_p^\gamma$.

The fact that the dominant terms are *central* suggests that the result must be common to forces of short but not zero range, though we have no simple argument explaining why $\mathcal{O}_p^\gamma$ should be so close to the schematic forms we have found. However, assuming that it is, there is a scaling argument that provides valuable insight into the $\mathcal{N}_p^\gamma$ denominator.

In leading order the expectation value of a Hamiltonian must go as the number of particles in the system. Therefore, in $\mathcal{H}$, the leading monopole terms must go as $O(A)$. As $\mathcal{H}_M$ will effectively act on one (or at most a small number of shells), the number of particles involved, and hence their energy, will be $O(D_f)=O(A^{2/3})$, where $D_f\approx p_f^2$ is the degeneracy of the Fermi shell. Since there are p_f possible multipole contributors, *each individual term must go as* $O(p_f)=O(A^{1/3})$, which—remembering that $\hbar\omega=40\,A^{-1/3}$ [20] —*is precisely what the normalized operators ensure, given the universal scaling provided by the* $\hbar\omega$ *factor*.

This statement demands a careful proof and we start by showing that the traditional choices for the pairing and quadrupole coupling constants produce empirical evidence in favor of the $O(A^{1/3})$ scaling for a given contribution, which we have suggested on heuristic grounds.

Consider first the pairing force. On a space of degeneracy D, it produces an energy

$$E_P=-\frac{|G|}{4}n(D-n+2)=-|G|O(nD).$$

The first equality is a standard result. Since $n=O(D_f)$, the conventional choice $G=O(A^{-1})$ can be interpreted as guaranteeing $E_P=O(A^{1/3})$. It is worth mentioning that the form of G was found empirically, and in a famous paper by Baranger and Kumar it is stated that''We know of no reliable way of predicting this A^{-1} dependence . . . '' [1]. The argument we have outlined provides a way that seems reliable.

For a quadrupole force, an estimate for the energy can be obtained by constructing a determinantal state that maximizes the quadrupole moment $Q_0=\Sigma_{i=1}^n(2n_{zi}-n_{xi}-n_{yi})$, where n_{xi}, n_{yi}, n_{zi} are the number of quanta. The largest term in the sum is then $2p$, the next $2p-3$, then $2p-6$, etc. Therefore $Q_0=O(np)$, and

$$E_q\approx-|\chi'|Q_0^2=-|\chi'|O(n^2D),$$

which in turn explains the origin of the usual choice $\chi'=O(A^{-5/3})$ for the quadrupole strength, which leads to $E_q=O(A^{1/3})$.

It is clear from Eqs. (2.9) and (2.10) that the operators are affected by coefficients that go as $A^{-1/3}D^{-1}$ (instead of A^{-1}) for pairing, and as $A^{-1/3}D^{-2}$ (instead of $A^{-5/3}$) for quadrupole. For $D=D_f$, the energies are again $O(A^{1/3})$, but now this important empirical fact is a direct consequence of the interaction. For arbitrary D, the energies of the traditional (old) form

$$E_{\text{old}} \Rightarrow E_P = O\left(\frac{nD}{A}\right), \quad E_q = O\left(\frac{n^2 D}{A^{5/3}}\right),$$

differ from those in the normalized version (new),

$$E_{\text{new}} \Rightarrow E_P = O\left(\frac{n}{A^{1/3}}\right), \quad E_q = O\left(\frac{n^2}{A^{1/3} D}\right).$$

If the n particles are promoted to some higher shell with $p_f = p_f + M$, $D \rightarrow (p+M)^2$, and both energies grow in the old version. For sufficiently large M, because of the term in M^2, the gain will become larger than the monopole loss, $O(nM\hbar\omega) = O(MA^{1/3})$, which is only linear in M. Therefore the traditional forces lead the system to collapse. If they are restricted to act in finite spaces, it is possible to obtain sensible results but the coupling constants must be reduced as the space is increased. (The problem will be discussed in Appendix C.) In the new form there is no collapse: E_P stays constant, E_q decreases, and the monopole term provides the restoring force that guarantees that particles will remain predominantly in the Fermi shell(s).

Although we have not given a formal proof of the generalization of Eqs. (2.9) and (2.10), the scaling arguments establish that it is physically sound, and that it is possible to 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 C).

The scaling arguments—so far applied to show that a realistic interaction has all the properties we expect on empirical grounds— can be turned around. Let us start with the assumption that the pairing plus quadrupole model must be true ''in some sense'' because of its explanatory power. Then we want to find an interaction that retains the model (i.e., separable forms), but does not lead to collapse. It is clear that with the single assumption of universal scaling, i.e., the validity of Eq. (2.8) and the $A^{1/3}$ dependence for the energies, we would obtain Eqs. (2.9) and (2.10), and their generalizations, or at least something very similar. Note in this respect that the normalizations are defined only to leading order $O(p^k)$, and we can say nothing about the $O(p^{k-1})$ terms, responsible for $\alpha^2 \neq 1$ in Eq. (2.7) and the slight differences we have neglected in the e and E couplings, but this is the good reason to neglect them.

One last remark. E_P and E_q contribute to what are commonly called ''shell'' effects. Although it seems clear that each individual contribution should go as $A^{1/3}$, it is not clear whether the total shell effects (including monopole) can add up to an $A^{2/3}$ behavior. For a discussion of this point see [12].

E. 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 MeV. Unsurprisingly it has the form $\Sigma n_p / \sqrt{D_p}$, which is what we expect of normalized operators, but it should be mentioned that there are several monopole candidates one can think of: the unit operator 1, which is identical to the number operator n in second quantization, but also r^2, for instance. When normalized they give the same result.

The remarkable thing about this form is that it provides the answer to an important problem raised in [7], which is that the monopole-monopole one naively expects as dominant, nn, 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 behavior 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 *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 [12], where a mass formula—of rather high precision by present standards—is derived.

III. CHOICE AND COMPLETE EXTRACTION OF H_C

There are two problems to be solved: what to extract from $\mathcal{H}$, and how to extract. The two subsections that follow are devoted to them.

A. Choice of H_C

The results so far invite a separation:

$$H = H_m + H_C + H_R,$$

where H_C is the collective or coherent part, while H_R is the rest. To define them with some precision, i.e., to decide what to extract, we shall rely on the result of Mon and French [19] that H_R could be viewed as random, as soon as its E distribution becomes symmetric.

The distributions will be characterized by their moments:

$$m_k = \frac{2}{D(D-1)} \sum (E^\Gamma)^k, \quad \gamma_1 = m_3 / m_2^{3/2},$$

and the vanishing of the skewness γ_1 will be seen to be sufficient to ensure symmetry. We use $m_2 = \sigma^2$.

Let us then define some cutoff ε, eliminate from H in the e representation those peaks with $|e_\gamma| > \varepsilon$, and decrease ε until the E distribution becomes symmetric. The result of the operation is shown in Figs. 3 and 4 for $\varepsilon = 2$ and 1.3 MeV, respectively. Labeling the original distribution in Fig. 1 as $(\varepsilon = \infty)$, we find the following moments (σ in MeV).

(i) $\varepsilon = \infty$, $\sigma^2 = 0.99$, $\gamma_1 = -2.22$. Since the lowest state $\Gamma = 1^+ 0$ is at -10.12 MeV its contribution to γ_1 is by far the largest but still only -0.61. It means that many states in the tail must contribute to m_3.

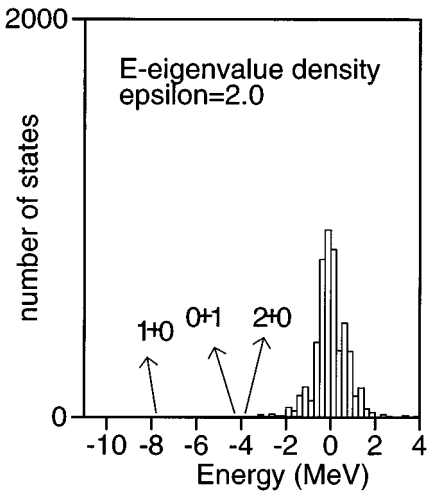

FIG. 3. E-eigenvalue density for the KLS interaction in the $pf+sdg$ major shells ($\hbar\omega=9$), after removal of the five largest multipole contributions. Each eigenvalue has multiplicity [Γ]. The largest ones are shown by arrows.

(ii) $\varepsilon=2.0$, $\sigma^2=0.60$, $\gamma_1=-0.79$. Five peaks have been excluded $\gamma=1^-0, 1^+1, 2^+0, 3^-0$, and 4^+0 and now the $\Gamma=1^+0$ state at -7.79 MeV accounts for most of γ_1 with a contribution of -0.60, which when added to that of the next two states $\Gamma=2^+0$ (-4.29 MeV) and 0^+1 (-3.82 MeV), at $\gamma_1=-0.86$, exceeds the full value. As anticipated, the very large e peaks 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 γ terms 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 Sec. V—must be counted as a nuisance, rather than a bona fide candidate to H_C.

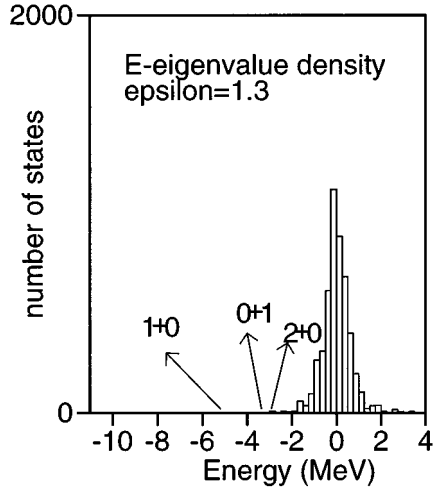

FIG. 4. E-eigenvalue density for the KLS interaction in the $pf+sdg$ major shells ($\hbar\omega=9$), after removal of multipole contributions with $|e|>$ 1.3. Each eigenvalue has multiplicity [Γ]. The largest ones are shown by arrows.

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

(iii) $\varepsilon=1.3$, $\sigma^2=0.41$, $\gamma_1=-0.002$. This cutoff was chosen as a sensible definition of the bulk of the e distribution. The histogramm in Fig. 4 now becomes structureless. The γ terms with $|e_\gamma|>1.3$ are listed in Table III. Some useful information is given, as their symmetry type [see Eqs. (A14) and (A15)], and their multipole nature whenever possible.

The cutoff is reasonable in that the majority of excluded peaks 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 cutoff (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, but in any case there are elements of guess, convenience, and trial and error in the choice, which is more of an art than a science, at least at present. The only safe prescription we can propose is to start with little—pairing plus quadrupole, say—and keep adding terms until it makes no difference.

If forced to take a more courageous stand, our choice would be the following.

(i) For the E terms we would only include pairing, i.e., the $\Gamma=01$ and 10 forces.

(ii) For the e terms the $\varepsilon=2$ cutoff sounds reasonable though it may be advisable to include also the insovector quadrupole term, which misses the cutoff but is coherent. In studies involving the giant dipole resonance the $\gamma=1^-1$ contribution is also called for of course.

The type of calculation has an influence on the attitude adopted.

As much as necessary applies to the recently developped shell-model Monte Carlo approach [13]. When the Hamiltonian is written in an e representation, 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. (A26b), and imagine that in V^{JT}_{rstu} the rs and tu states are allowed to be symmetric. The linear dependence problem is solved, but as 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 is costly and something like the $\varepsilon=1.3$ cutoff may be necessary. (At the end of the next subsection there is a comment relevant to this question.)

The alternative is to include pairing in the E representation, which is technically feasible [21]. The problem becomes much simpler, and for the e terms the $\varepsilon=2$ cutoff with the provisos mentioned above is a choice worth considering.

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 recent study [22], it is shown that states of four neutrons and four protons moving in the same or contiguous major shells generate rota-

tional spectra exhibiting systematic backbending. With a proper choice of coupling constant a $\overline{q\cdot q}$ force leads to wave functions that 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 is calculated using the $\overline{q\cdot q}$ eigenvectors, the spectrum reproduces perfectly the exact one. The example indicates that ''as little as possible'' may be little indeed, with lowest order perturbation theory supplying the necessary improvements.

This example is particularly relevant because the ''proper'' quadrupole strength that reproduces best the exact results is some 30% larger than e eigenvalue in Table III. 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 reason that explains the increase in the coupling constant, as explained next.

B. Complete extraction

At this point we may have a good idea about *what* to separate, but since most of it comes from a multipole representation, to decide exactly *how*, we must realize that H_C and H_R are ''orthogonal'' by construction in the multipole representation, but they need not be in the the normal one. The notion of orthogonality is important and demands a digression.

The complete symmetry that the equations indicate between the ω^{γ}_{rtsu} and W^{Γ}_{rstu} matrix elements is fictitious, because the latter must be antisymmetric in the indices rs and tu, while no restrictions apply to the former. To understand the problem raised by this situation we note that V in Eq. (A20) is invariant with respect to the choice of orderings because of Eqs. (A18b), while V in Eq. (A21) or (A23) will *look* very different for different orderings. Of course, it will always be the same object, which means that a given operator in the multipole representation can be written in terms of other operators apparently unrelated to it. This ambiguity may occasionally allow some freedom in the choice of forms of V, but in general we need to eliminate the ambiguities rather than take advantage of them, as can be seen from the following argument. Let us assume some very simple force such as quadrupole-quadrupole $(q\cdot q)$, and take it to normal form. The symmetric matrix elements will disappear since they are associated to operators that vanish identically. Now transform back to the multipole representation: The operator will no longer look like $q\cdot q$, but it will still be the original one. But then, since an operator may have different guises, how to decide what it *really* is?

The only solution is to refer always to the normal form, which is unique. Therefore what is needed is a way to compare two Hamiltonians H_A and H_B, defined in some finite space by their matrix elements V^{Γ}_{rstuA} and V^{Γ}_{rstuB}. Intuitively, the thing to do is treat these two sets as components of vectors, and introduce a scalar product remembering that for each Γ we have $[\Gamma]$ components:

$$H_A\cdot H_B=\sum\,[\Gamma]V^{\Gamma}_{rstuA}V^{\Gamma}_{rstuB}\,. \tag{3.1}$$

This tentative definition, already suggested in [15], was substantiated in [23]. Since this paper is hard to follow, we propose two arguments to suggest the validity of (3.1). The first is purely heuristic.

Let us assume some H_B that we want to separate from the full Hamiltonian H. The problem can be stated by writing

$$H=(H-\lambda H_B)+\lambda H_B\equiv H_A+H_B \tag{3.2}$$

and by demanding that $(H-\lambda H_B)^2$ be as small as possible. Since we are dealing with an operator, ''small'' must be interpreted in an average sense. It is equivalent to saying that the ''size'' or ''norm'' of an operator must be defined through the trace of its square, and therefore we want to minimize

$$\mathrm{Tr}[(H-\lambda H_B)^2]=\sum_{rstu\Gamma}[\Gamma](V^{\Gamma}_{rstu}-\lambda V^{\Gamma}_{rstuB})^2. \tag{3.3}$$

The minimum we are after is found to be at

$$\lambda=\sum_{rstu\Gamma}[\Gamma]V^{\Gamma}_{rstu}V^{\Gamma}_{rstuB}\Big/\sum_{rstu\Gamma}[\Gamma](V^{\Gamma}_{rstuB})^2$$
$$\equiv H\cdot H_B/H_B\cdot H_B\,.$$

It can be easily checked that this is equivalent to

$$H_A\cdot H_B=0.$$

To meet the demand after Eq. (3.2), H_A and H_B must be made ''as different as possible'' which amounts to making them orthogonal in the sense of Eq. (3.1).

The second argument in favor of the definition in (3.1) is simple but strong: the norms associated with each representation can be used to define product norms for the Hamiltonians since each matrix element affects an operator that is quadratic in the ''unit vectors'' Z_{rs} and S_{rs}. For the E representation, the product norm is identical to the one introduced in Eq. (3.1).

Turning to our specific problem, the simplest thing to do is to orthogonalize H_C and H_R through

$$H_R+H_C=\left(H_R-\frac{H_C\cdot H_R}{H_C\cdot H_C}H_C\right)+H_C\left(1+\frac{H_C\cdot H_R}{H_C\cdot H_C}\right).$$

By squaring we find

$$\left[H_R\cdot H_R-\frac{(H_C\cdot H_R)^2}{(H_C\cdot H_C)}\right]+\left[H_C\cdot H_C+2H_C\cdot H_R+\frac{(H_C\cdot H_R)^2}{(H_C\cdot H_C)}\right].$$

If $(H_C\cdot H_R)^2/(H_C\cdot H_C)$ can be neglected, the orthogonalization amounts to leaving H_R untouched, and to boosting H_C by the cross term. Now we call upon Eq. (B6), which says that the total norms in the two representations are proportional, and examine the relative contributions of H_C and H_R in both cases.

For $\varepsilon=2$, from Table III we can find that the five largest peaks contribute 0.29, i.e., some 30% to the total norm which we know to be 0.99, and therefore H_R accounts for the remaining 70%. But we also know that, when calculated in the normal representation, H_R^2 is not 0.70, but 0.60, and therefore the orthogonalization boosts the share of H_C to 40%, which implies a $\sqrt{4/3}\equiv 15\%$ 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.

Assume we have selected the candidates to H_C. Call them H_κ and transform the multipole ones to the normal representation. We want to find the linear combination $H_C=\Sigma C_\kappa H_\kappa$ that maximizes the overlap between H_C and H. It amounts to a standard minimization of the expression ($\alpha\equiv rstu$)

$$\sum_\alpha \left(W^\Gamma_\alpha - \sum_\kappa C_\kappa W^\Gamma_{\alpha\kappa} \right)^2 [\Gamma] = \left(H - \sum_\kappa C_\kappa H_\kappa \right)^2$$

$$= H\cdot H - 2\sum_\kappa C_\kappa H_\kappa \cdot H + 2\sum_{\kappa,\kappa'} C_\kappa C_{\kappa'} H_\kappa \cdot H_{\kappa'}, \tag{3.4}$$

and therefore C_κ is determined by the linear system

$$H_\kappa \cdot H = \sum_{\kappa'} H_\kappa \cdot H_{\kappa'} C_{\kappa'}. \tag{3.5}$$

The C_κ coefficients are uniquely defined provided the H_κ operators are linearly independent. Each H_κ can be written in the representation best adapted to the calculation at hand.

It may be of interest to make them orthogonal by diagonalizing the norm matrix $H_\kappa \cdot H_{\kappa'}$ through transformation $T_{\mu\nu}$:

$$H_\mu = \sum T_{\mu\kappa} H_\kappa, \quad H_\kappa = \sum T_{\kappa\mu} H_\mu,$$

$$H_\mu \cdot H_{\mu'} = \delta_{\mu\mu'} H^2_\mu. \tag{3.6}$$

Therefore, defining H_C in terms of the H_μ, we have

$$H_C = \sum C_\mu H_\mu \overset{(3.5)}{\Rightarrow} C_\mu = H_\mu \cdot H / H^2_\mu. \tag{3.7}$$

A potentially interesting result is worth mentioning. In the *sd* shell we have included in H_C the strongest contribution for each γ plus the pairing terms. In solving Eq. (3.5) it turns out that the exclusion of the latter makes a negligible difference.

IV. CORE POLARIZATION AND EFFECTIVE CHARGES

To be of use in a shell-model calculation, the Hamiltonian (and other operators) must be renormalized to account for the effect of states outside the model spaces in which we are prepared to work. When realistic matrix elements were introduced, the necessity of this operation was immediately recognized, and by using a simple perturbative prescription, Kuo and Brown (KB) were able to obtain numbers that agreed quite nicely with the spectra of ^{18}O and ^{18}F [24]. The agreement was so good that it led to much research trying to establish whether it was fortuitous or genuine. After some 30 years, it appears that it is quite genuine, and a recent calculation [25], using far more sophisticated techniques and more modern interactions than those of [24], produces very much the same results, as will be illustrated in Sec. V. The state of the art on the subject of renormalizations is discussed in a recent review article [26].

In this section we shall calculate effective coupling constants for the pairing and quadrupole forces in second order perturbation theory, which will be seen to be very close to those extracted from [25], and to the empirically determined ones. Satisfactory effective charges will also be obtained by repeating, with a realistic force, exactly the steps followed by Mottelson in his classical derivation [27]. The simplicity of the derivation may be of help in understanding the difficulties encountered in the standard approaches to quadrupole polarizability [28] (see, however [29], for a more successful calculation using a Skyrme force).

Before going into the calculations it is worth explaining why, for the energies, it seems possible to obtain, in second order perturbation theory, results close to those of the standard formulations that go to higher orders. In [26] it is explained how to go about constructing a good G matrix with a good potential, and then solving the problems raised by the perturbative expansion with as much rigor as possible. However, it has been claimed for a long time that it is dangerous to be too rigorous with an interaction that is known to have bad saturation properties [30], and this is why the monopole-multipole separation strategy has been adopted. As it happens, we have been lucky, because *the serious problems that need careful consideration in a rigorous perturbative approach seem to have a monopole origin.* This was hinted in [30], and here we offer two further plausibility arguments borrowed from [25] and [26].

(1) Many of the difficulties in the standard treatments are related to the tensor force. In our case these problems do not exist because the perturbation is caused by $\mathcal{H}_M$ which is a *central* interaction for the dominant terms of interest.

(2) Higher order corrections become less important if a Hartree-Fock basis is used. Again a monopole effect.

Another argument in favor of low order perturbative corrections comes from [31], where diagonalizations in the full pf shell are treated in second order using as unperturbed states the $f^n_{7/2}$ configurations. Exact results [10] have confirmed the validity of the approach. The test passed by second order estimates is seen to be very stringent because a $0\hbar\omega$ space is involved, with denominators much smaller than the typical $2\hbar\omega$ we shall encounter now. However, the test applies only to finite vector spaces. If the whole Hilbert space is probed problems may (and will) arise.

We shall use the quasiconfiguration method, which provides a flexible framework, and is particularly well adapted to diagonal representations [31–33]. The idea is to separate the full space into a model part 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

$$|\overline{i}\rangle = |i\rangle + \sum_j A_{ij}|j\rangle, \quad |\overline{J}\rangle = |j\rangle - \sum_i A_{ij}|i\rangle,$$

which respects strict orthogonality:

$$\langle \overline{\imath}\,|\overline{J}\rangle = 0.$$

The amplitudes A_{ij} are then defined by

$$\langle \overline{\imath}|\mathcal{H}|\overline{J}\rangle = 0,$$

which leads to a set of coupled equations defining the effective interaction in its most general form. In particular, linked cluster perturbation theory follows from Neumann expansion, and diagrammatic techniques may be introduced if necessary, but are not essential. We refer to [31–33] for fuller information, and we simply borrow from these references the expressions for the second order corrections, and apply them in some detail to the pairing and quadrupole Hamiltonians.

The use of diagonal representations makes the calculations analytic, and it will become clear how the quasiconfiguration method transforms the dressing of the states into the dressing of the operators. It should be noted, however, that the second order results should be identical to what would be obtained with the conventional (m-scheme) methods.

A. Pairing

We deal first with the effect on shell p of shell $p+1$ only. E_{01} is a one-shell energy from Table II, scaled by $\hbar\omega/\hbar\omega_0$, and $\hbar\omega_0 = 9$ MeV (for typographical reasons we shall use E_{01} instead of E^{01}):

$$\langle \overline{\imath}|H_P^{\dagger}|\overline{\imath'}\rangle = \left\langle i \left| E_{01}(\omega)\frac{P_p^{\dagger}\cdot P_p}{\Omega_p}\right| i'\right\rangle \tag{4.1a}$$

$$-\frac{E_{01}^2(\omega)}{2\hbar\omega}\sum_J \frac{\langle i|P_p^{\dagger}\cdot P_{p+1}|J\rangle\langle J|P_{p+1}^{\dagger}\cdot P_p|i'\rangle}{\sqrt{\Omega_p\Omega_{p+1}}\sqrt{\Omega_p\Omega_{p+1}}} \tag{4.1b}$$

$$= \left\langle i \left| E_{01}(\omega)\frac{P_p^{\dagger}\cdot P_p}{\Omega_p} - \frac{E_{01}^2(\omega)}{2\hbar\omega}\frac{1}{3}\frac{P_p^{\dagger}\cdot P_p}{\Omega_p}\frac{P_{p+1}\cdot P_{p+1}^{\dagger}}{\Omega_{p+1}}\right| i'\right\rangle \tag{4.1c}$$

$$= \left\langle i \left| E_{01}(\omega)\left(1-\frac{E_{01}(\omega)}{2\hbar\omega_0}\right)\frac{P_p^{\dagger}\cdot P_p}{\Omega_p}\right| i'\right\rangle. \tag{4.1d}$$

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 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},

$$E_{01}\to E_{01}\left(1+\frac{|E_{01}|(\omega)}{\hbar\omega}\right)\equiv E_{01}\to E_{01}(1+0.32). \tag{4.2}$$

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

$$E_{01}(\omega)\left[1+\frac{|E_{01}(\omega)|}{2\hbar\omega}\left(1+\frac{1}{2}+\frac{1}{3}+\cdots\right)\right], \tag{4.3}$$

$$G\left[1+\frac{|G|}{2\hbar\omega}\left(\Omega_{p+1}+\frac{\Omega_{p+2}}{2}+\frac{\Omega_{p+3}}{3}+\cdots\right)\right]. \tag{4.4}$$

The normalization of the operators P_p transforms a very bad divergence into a logarithmic one, which is still a divergence.

The problem may be due to a fault in our formulation. It is possible, for instance, that since high-lying pairing excitations violate badly translation invariance the corresponding matrix elements should be quenched and this could be perhaps sufficient to eliminate the divergence. It is also true that what we treat as a potential is a G matrix, and in earlier work it was argued that the perturbative treatment leads to double counting, but it can be shown that lowest order Brueckner theory amounts to discarding the short range repulsion and replacing it by a density-dependent saturating mechanism [33]. Therefore, it should be possible to treat a G matrix as a smooth potential, but then the postulated form for the pairing term may not be correct.

However, it may also be that the logarithmic divergence is a real problem that has to be solved by doing better than second order perturbation theory, and the simplicity of the Hamiltonian makes it possible to push the exploration very far. We have here an illustration of the efficacy of the diagonal representations in transforming a toy model into what may be a reasonably realistic one.

B. 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 is due to $2\hbar\omega$ jumps mediated by a term of the form $k(\overline{q_p'}\cdot\overline{q_{2\hbar\omega}'}+\overline{q_{2\hbar\omega}'}\cdot\overline{q_p'})$, which must be extracted from $\mathcal{H}_M$. 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 B under the item *Asymmetric factorization*. The space involves all shells from $p=0$ to 4, and the matrix elements we are not interested in are eliminated (those of the form $\overline{q_{2\hbar\omega}'}\cdot\overline{q_{2\hbar\omega}'}$). 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 $\overline{q_p}\cdot\overline{q_{p+1}}$ component. To compare with empirical reults in the sd, $p=2$ shell we work at $\hbar\omega=11$. The standard one shell calculation yields $e^{20}=-2.40$ MeV [note that Eq. (C3) gives -2.37 MeV]. For the cross terms the large matrix produced

$$k=-2.80 \text{ MeV}, \quad \langle\overline{q_2'}|\overline{q_2}\rangle = 0.97, \tag{4.5}$$

$$\langle\overline{q_{2\hbar\omega}'}|q_{02}+q_{13}+q_{24}\rangle/\mathcal{N}_{2\hbar\omega} = 0.83, \tag{4.6}$$

where $q_{pp'}$ are the $2\hbar\omega$ quadrupole operators that can couple to q_2. Their sum is normalized to $\mathcal{N}_{2\hbar\omega}$. By normal-

izing each $q_{pp'}$ operator separately the overlap at 0.87 is slightly better, but it is the number in Eq. (4.6) we shall need.

From Eq. (4.5), $\overline{q_2'} \approx \overline{q_2}$, and this is important because the closeness of $\overline{q_2'}$ to $\overline{q_2}$ ensures that ''quadrupole renormalizes quadrupole'' and that effective charges are state independent as shown below.

Proceeding as in Eqs. (4.1), we have (H.c. stands for Hermitean conjugate of the first term)

$$\langle \overline{i}|H_{\overline{q}}|\overline{i'}\rangle = e_{20}(\omega)\langle i|\overline{q_p}\cdot\overline{q_p}|i'\rangle \tag{4.7a}$$

$$-\frac{k^2(\omega)}{2\hbar\omega}\langle i|(\overline{q'_{2\hbar\omega}}\cdot\overline{q_p}+\text{H.c.})|J\rangle\langle J|(\overline{q'_{2\hbar\omega}}\cdot\overline{q_p}+\text{H.c.})|i'\rangle \tag{4.7b}$$

$$\cong\left\langle i\left|e_{20}(\omega)\overline{q_p}\cdot\overline{q_p}-\frac{2k^2(\omega)}{\hbar\omega}\frac{1}{5}\overline{q'_{2\hbar\omega}}\cdot\overline{q'_{2\hbar\omega}}\overline{q_p}\cdot\overline{q_p}\right|i'\right\rangle \tag{4.7c}$$

$$=\left(e_{20}(\omega)-\frac{k^2(\omega)}{\hbar\omega}\right)\langle i|\overline{q_p}\cdot\overline{q_p}|i'\rangle. \tag{4.7d}$$

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 $q'_{2\hbar\omega}\equiv q'_{p-2p}+q'_{p-1p+1}+q'_{pp+2}$ as commuting with $\overline{q_p}$, 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 [31] in which a very similar case is fully worked out. The neglect of three-body contributions is common, but bad, practice.

1. Effective charges

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

$$\langle\overline{i|q|i'}\rangle=\langle i|q_p|i'\rangle-\frac{2k(\omega)}{2\hbar\omega}\langle i|q_{2\hbar\omega}(\overline{q'_{2\hbar\omega}}\cdot\overline{q_p}+\text{H.c.})|i'\rangle \tag{4.8a}$$

$$=\langle i|q_p|i'\rangle-\frac{2k(\omega)}{\hbar\omega}\frac{1}{5}\frac{\mathcal{N}_{2\hbar\omega}}{\mathcal{N}_p}\langle i|q_p\overline{q_{2\hbar\omega}}\cdot\overline{q'_{2\hbar\omega}}|i'\rangle \tag{4.8b}$$

$$=\left(1-0.83\frac{k(\omega)}{\hbar\omega}\frac{\mathcal{N}_{2\hbar\omega}}{\mathcal{N}_p}\right)\langle i|q_p|i'\rangle. \tag{4.8c}$$

What we have done is (a) use the second order expression and (b) upon recoupling collect two 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.

This second order estimate of the effective quadrupole operator is equivalent to Mottelson's [27], which was made using a conventional $k'q\cdot q$ force. Then, in step (b) above the quotient of the norms $\mathcal{N}_{2\hbar\omega}/\mathcal{N}_p$, does not appear, and the final result changes to

$$\langle\overline{i|q|i'}\rangle\overset{[27]}{=}\left(1-\frac{k'(\omega)}{\hbar\omega}\mathcal{N}^2_{2\hbar\omega}\right)\langle i|q_p|i'\rangle, \tag{4.9}$$

a factor $\mathcal{N}^2_{2\hbar\omega}$ appearing now because the contraction $\langle i|q_{2\hbar\omega}\cdot q_{2\hbar\omega}|i'\rangle$involves unnormalized operators.

For $p=2$ we obtain $\mathcal{N}_{2\hbar\omega}/\mathcal{N}_p=1.97$, which turns out to be very close to the value for large p that can be calculated with the help of Eqs. (A33) and (A34). Taking as coupling constants $k(\omega)=-2.8\hbar\omega/11$ and $k'=-\hbar\omega/(8\mathcal{N}_p^2)$ (see after last equation of Appendix B), the transition operator is boosted by a factor $(1+0.42)$ for Eq. (4.8), and $(1+0.5)$ for Eq. (4.9), which are 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 ([31] contains some examples). It is argued in [27] that a resummation to all orders in perturbation theory [random phase approximation (RPA)] is necessary, and that it amounts to recognizing that the 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 $Q^{20}=(1+x)q^{20}$ ($x=0.42$ or 0.5) becomes

$$Q^{20}=q^{20}+xQ^{20}\rightarrow Q^{20}=(1-x)^{-1}q^{20}.$$

Mottelson also argues that x corresponds to the mass polarizability of the system, and that for the $E2$ operator it should be replaced by $x\rightarrow xZ/A$. However, the quasiconfiguration technique we have used makes it clear that x is the isoscalar polarizability, and what is needed is a similar calculation for the isovector one. The steps are as in Eqs. (4.8); all numbers are the same except for the coupling, which is now $k=+1.28$ MeV.

C. Comparisons

For the sd shell, precise empirical data can be compared with the calculated effective coupling constant and effective charges η^{20} and η^{21}. The numbers are (e^{20} in MeV)

$$e^{20}\rightarrow e^{20}(1+0.3)=-3.12 \text{ vs } -3.18\ [34], \tag{4.10}$$

$$\eta^{20}=(1-0.42)^{-1}=1.76 \text{ vs } 1.78(3)\ [6], \tag{4.11}$$

$$\eta^{21}=(1+0.19)^{-1}=0.8 \text{ vs } 0.8(1)\ [6]. \tag{4.12}$$

The quality of the agreement is pleasing, and e^{20} is also close to the Bonn B value given in Table V (-3.32 MeV).

In principle the effective charges above should be valid for all regions, provided Eqs. (4.8) scale well. We have mentioned in this respect that $\mathcal{N}_{2\hbar\omega}/\mathcal{N}_p$ seems independent of p, but we have neither checked the constancy of the overlap factor (0.83) nor the linearity of $k(\omega)$. Furthermore, we have to remember that the choice of energy denominators at $2\hbar\omega$ is at best a good average, since the isoscalar states must be below the isovector ones. All these uncertainties amount to changing x by a multiplicative factor, and to have an idea of their impact we simply replace the overlap factor of 0.83 by one (in which case the isoscalar polarizability coincides with Mottelson's). The effective charges for protons and neutrons [i.e., $(\eta^{20}\pm\eta^{21})/2$], which are $e_\pi=1.31$ and

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. ← 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←
5153	20	-1.10	-1.44	-1.33	-0.1 ←

$e_\nu=0.46$ in Eqs. (4.11) and (4.12), would become $e_\pi=1.41$ and $e_\nu=0.60$. It is seen that the uncertainties are likely to have small effects.

The comparison of the effective pairing numbers in Eq. (4.2) with empirical values would show that we are missing some strength. Going up to $4\hbar\omega$ jumps leads to an effective energy (in MeV)

$$E_{01}\rightarrow E_{01}(1+0.48)=-5.4 \text{ vs } -5.7 \text{ [34]}.$$

The agreement with Bonn B in Table V (-5.5 MeV) is also good, but we should remember that the logarithmic divergence of second order theory is still there.

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 [26]).

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. The calculations that generated the controversies were done in the sd shell, a region where quadrupole and hexadecapole are already high multipolarities, well represented in the pairing decomposition (see last paragraph in Sec. III). Therefore, their strong polarizabilities will have a non-negligible effect on the $\Gamma=01$ matrix elements. This is simply a manifestation of the linear dependence problem we have often encountered.

In heavier nuclei the important contributions to H_C will become increasingly orthogonal, and they will increasingly renormalize themselves in a strict sense.

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 larger, and neglect the small ones that have no chance to grow.

V. 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 IV shows some off-diagonal matrix elements at the beginning of the shell, calculated with the KLS (as used in [9]), KB [24], and Bonn B [25] realistic interactions, or taken from the W fit. The KLS numbers represent bare matrix elements affected by a multiplicative factor of 1.4 for $T=1$. This extremely coarse ''renormalization'' will be seen to be quite acceptable. 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 shown by arrows.

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 V 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 deserves some attention. It shows mainly in the lower half of the region, and we borrow from unpublished results used in the calculations of [9] some of the following observations.

(1) In ^{22}Na the realistic interactions produce a close doublet $J=1$, 3, instead of the well detached $J=3$ observed ground state. Reference [6] contains a useful figure for this nucleus. Monopole corrections very much improve—but not completely—the catastrophic behavior of the realistic inter-

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

01	10	20	30		10	11	20	21	30	31	40	41
-5.42	-5.43	-2.68	-2.15	KLS	-2.18	2.38	-2.90	-0.71	-0.82	0.44	-1.61	0.40
-5.48	-6.24	-2.91	-2.66	Bonn B	-1.55	2.64	-3.32	-0.97	-0.83	0.46	-1.39	0.52
-5.69	-5.90	-0.95	-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	$\langle$KLS$\vert$Bonn B$\rangle$	0.99	1.00	1.00	0.99	0.98	0.99	1.00	1.00
1.00	0.98	0.55	0.82	$\langle$KLS$\vert$ $W\rangle$	0.95	0.99	1.00	0.98	0.98	0.92	1.00	1.00

actions indicated by the figure.

(2) The $k=3/2$ band in ^{23}Na is too low.

(3) The γ band in ^{24}Mg is also too low.

(4) The $JT=20$ state in ^{18}F always too low by about 1 MeV. This seems to be true for all interactions [25]. (One should be careful here: The experimental counterpart of this level is the second $JT=20$ state in ^{18}F, the first one is an intruder.) In ^{38}K, the $JT=20$ state (which is now the first) is again too low. This will turn out to be a most interesting indication, because in the upper part of the shell the realistic interactions do extremely well, and this state is the one of the very few that causes trouble.

These discrepancies are very mild when compared with the ones due to bad monopole behavior but they are mostly responsible for the fact that the best results quoted in [9] give rms errors of some 100 keV above the W values.

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. It is quite possible that monopole effects are still responsible for the discrepancies, but it is worth examining whether the multipole terms may be at fault.

One possibility is that the renormalizations are not correct: What was said for pairing in the preceding section applies to all the strong Γ contributions.

The other possibility is to exploit the differences between realistic interactions. Similar as they are, they also differ in some respects as can be gathered from Fig. 3 of Ref. [25], which shows several calculated spectra of ^{18}F and ^{18}O.

There are two effects.

(i) Overall dilation. If we refer to Eq. (2.8), 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 differences due to this phenomenon can be eliminated by normalizing the interactions to the same σ^2 in Eq. (3.1). When this is done, most of the discrepancies between interactions in Fig. 3 of Ref. [25] will be removed.

(ii) Spectroscopically light matrix elements. The interactions would still differ, especially through the ''spectroscopically light'' matrix elements, i.e., those of small $[JT]$, and in particular the $JT=01$ and 10 ones. As we have seen in the preceding section they are also the ones most severely affected by renormalization uncertainties.

These remarks suggest ways of attacking the local problem in the sd shell. From Table V it is clear that there is no room whatsoever for tampering with the structure (i.e., the wave functions) of the dominant terms. The magnitudes of the energies are more flexible. Since the $JT=20$ state has been clearly identified as a troublemaker, it has to be moved up. Or, conversely, the states below it in the two particle (or hole) spectra must be moved down. Monopole terms can then correct the overall energetic balance: The important Γ states have different particle occupancies, and are quite sensitive to monopole details. As the radial behavior of nuclei in the first half of the shell is very complicated [9], the effective H_m may also be complicated and accomodate E^Γ values quite different from those in Table V, which are already somewhat scattered. The differences may come either from better renormalizations or from the interactions themselves. The latter prospect is an interesting one, since it may help in choosing interactions: Our basic tenet that the realistic ones are equivalent is basically sound, but not strictly true.

The local problem remains, but the diagonal representations put useful constraints on the possible solutions. More generally, our analysis has confirmed that there is not much room for tampering with the realistic interactions.

VI. CONCLUSION

The residual or multipole part of the nuclear Hamiltonian is dominated by few terms that are very simple. Work remains to be done on the monopole field, but as things stand, we have already a fairly useful characterization of the interaction.

APPENDIX A

1. Basic operators

We shall work in spaces containing D orbits labeled (rr_z), (s,s_z) . . . , where r specifies the subshell to which the orbit belongs, and r_z its projection quantum numbers. The associated creation $(a^\dagger_{rr_z})$ and annihilation (a_{rr_z}) operators obey anticommutation relations.

All operators we may need are products of these elementary ones and, to take advantage of the basic symmetries, they have to be coupled to good angular momentum J (j formalism), or to both good J and isospin T (jt formalism). Following French [15], we shall introduce a product notation in which expressions are independent of the coupling scheme. In jt formalism, for example, a single tensorial index will represent pairs in spin-isospin (JT) space:

$$\Gamma\equiv JT,\ \ \Gamma_z\equiv MT_z,\ \ r\equiv j_r\tfrac{1}{2},\ \ r_z\equiv m_r\tau_{z_r},\ \text{ etc.} \quad \text{(A1)}$$

Note that r as tensor index has not exactly the same meaning as label of shell r (i.e., $r\equiv j_r p_r$, where p_r is the principal quantum number). No confusion can possibly arise from this convention.

Expressions involving these indices will stand for products as in

$$(-)^{\Gamma_z}=(-)^{M+T_z},\quad (-)^r=(-)^{j_r+1/2},\quad [r]=2(2j_r+1),$$

$$[\Gamma]=[JT]=(2J+1)(2T+1), \quad \text{(A2)}$$

more generally

$$U(\Gamma\text{ space})=U(J\text{ space})U(T\text{ space}), \quad \text{(A3)}$$

where U may be some $6j$ or Clebsh-Gordan coefficient or similar functions as in

$$\langle\gamma\gamma_z\gamma'\gamma'_z|\Gamma\Gamma_z\rangle=\langle jmj'm'|JM\rangle\langle tt_zt't'_z|TT_z\rangle. \quad \text{(A4)}$$

In j formalism, also called neutron-proton (np), we do not couple explicitly to good T, the tensorial indices refer to a single space, and the identifications are $\Gamma=J$, $r\equiv j_r$, $[r]=(2j_r+1)$, etc. (Note that when used as label, r must specify whether the shell is a neutron or a proton one.)

The Hermitian conjugate (denoted by an asterisk *) of a tensor operator $\mathcal{T}$ is not itself a good tensor but it can be associated to one, which may be its ''conjugate'' $\widetilde{\mathcal{T}}$ or its ''adjoint'' $\overline{\mathcal{T}}$, whose components are defined by

$$\widetilde{\mathcal{T}}_{\gamma\gamma_z}=(-)^{\gamma+\gamma_z}(\mathcal{T}_{\gamma-\gamma_z})^*, \quad \overline{\mathcal{T}}_{\gamma\gamma_z}=(-)^{\gamma-\gamma_z}(\mathcal{T}_{\gamma-\gamma_z})^*. \tag{A5}$$

The $(-)^{\gamma}$ factor is not essential, and in the case of the spherical harmonics with the Condon-Shortley phase, for which $Y^*_{lm}=(-)^l Y_{l-m}$, there is no point in introducing it. On the contrary, the $(-)^{\pm\gamma_z}$ phase is dictated by the definition of tensor operators [see Eq. (4.9) and Sec. 4.8 of [16]], and the ambiguity in sign demands some care.

In coupling operations it is convenient to adopt the notation of French for the basic fermions:

$$A_{rr_z}=a^{\dagger}_{rr_z}, \quad B_{rr_z}=\tilde{a}_{rr_z}=(-)^{r+r_z}a_{r-r_z}. \tag{A6}$$

The *coupled* operators quadratic in A and B are

$$X^{\dagger}_{\Gamma\Gamma_z}(rs)=(A_rA_s)^{\Gamma}_{\Gamma_z}, \quad X_{\Gamma\Gamma_z}(rs)=(B_rB_s)^{\Gamma}_{\Gamma_z},$$

$$S^{\gamma}_{\gamma_z}(rt)=(A_rB_t)^{\gamma}_{\gamma_z}. \tag{A7}$$

The notation $X^{\dagger}_{\Gamma\Gamma_z}(rs)=X^{\dagger}_{rs\Gamma\Gamma_z}$ (and similar ones for the other operators) will be also used.

From the easily proved identity valid for any two operators,

$$(\overline{P^{\gamma}Q^{\gamma'}})^{\Gamma}=(-)^{\gamma+\gamma'-\Gamma}(\overline{Q}^{\gamma'}\overline{P}^{\gamma})^{\Gamma} \tag{A8}$$

(equally valid for conjugation), we obtain

$$\overline{X^{\dagger}_{\Gamma}}(rs)=-X_{\Gamma}(rs), \quad \overline{S^{\gamma}_{\gamma_z}}(rt)=(-)^{t-r-\gamma}S^{\gamma}_{-\gamma_z}(tr). \tag{A9}$$

For reduced matrix elements we use Racah's definition

$$\langle\alpha\alpha_z|P^{\gamma}_{\gamma_z}|\beta\beta_z\rangle=(-)^{\alpha-\alpha_z}\begin{pmatrix}\alpha & \gamma & \beta\\ -\alpha_z & \gamma_z & \beta_z\end{pmatrix}\langle\alpha\|P^{\gamma}\|\beta\rangle. \tag{A10}$$

Note that the reduction applies to both spin and isospin if we are working in a jt formalism. For any operator P^{γ} it is true that

$$\langle\alpha\alpha_z|P^{\gamma}_{\gamma_z}|\beta\beta_z\rangle=\langle\beta\beta_z|(P^{\gamma}_{\gamma_z})^*|\alpha\alpha_z\rangle^* \tag{A11}$$

and by applying Eq. (A10) to both sides it follows that

$$\langle\alpha\|P^{\gamma}\|\beta\rangle=(-)^{\alpha-\beta-\gamma}\langle\beta\|\overline{P^{\gamma}}\|\alpha\rangle, \tag{A12}$$

where we have omitted complex conjugation on the right-hand side (RHS) because our reduced matrix elements will be real.

The coupled form of a rank 1 operator is deduced from the uncoupled one by using Eq. (A10) and the definition of S^{γ} in (A7):

$$R^{\gamma}_{\gamma_z}=\sum_{r,t,r_z}\langle rr_z|R^{\gamma}_{\gamma_z}|tt_z\rangle a^{\dagger}_{rr_z}a_{tt_z}$$

$$=\sum_{rt}\langle r\|R^{\gamma}\|t\rangle(\gamma)^{-1/2}S^{\gamma}_{\gamma_z}(rt). \tag{A13}$$

We can always rewrite an arbitrary R^{γ} in terms of symmetric ($\mathcal{S}$) and antisymmetric ($\mathcal{A}$) operators:

$$R^{\gamma}_{\gamma_z}=\frac{1}{2}\sum_{r\leqslant t}\{[R^{\gamma}_{rt}+(-)^{r-t}R^{\gamma}_{tr}]\mathcal{S}^{\gamma}_{\gamma_z}(rt)$$

$$+[R^{\gamma}_{rt}-(-)^{r-t}R^{\gamma}_{tr}]\mathcal{A}^{\gamma}_{\gamma_z}(rt)\}, \tag{A14}$$

where we have used $R^{\gamma}_{rt}=\langle r\|R^{\gamma}\|t\rangle(\gamma)^{-1/2}$, and

$$\mathcal{S}^{\gamma}_{\gamma_z}(rt)=S^{\gamma}_{\gamma_z}(rt)+(-)^{r-t}S^{\gamma}_{\gamma_z}(tr),$$

$$\mathcal{A}^{\gamma}_{\gamma_z}(rt)=S^{\gamma}_{\gamma_z}(rt)-(-)^{r-t}S^{\gamma}_{\gamma_z}(tr). \tag{A15}$$

The $(-)^{r-t}$ phase ensures that the spherical harmonics are symmetric if $Y^*_{lm}=(-)^m Y_{l-m}$ (Condon and Shortley's choice), which leads to $\langle r\|Y_l\|t\rangle=(-)^{r-t}\langle t\|Y_l\|r\rangle$ and vanishing of the $\mathcal{A}$ term. The phase convention should be changed to $(-)^{r-t-l}$ if $Y_l\rightarrow i^l Y_l$. Then $Y^*_{lm}=(-)^{l+m}Y_{l-m}$, and $\langle r\|Y_l\|t\rangle=(-)^{r-t-l}\langle t\|Y_l\|r\rangle$. Note that now $Y_l\cdot Y_l=[l]^{1/2}(Y_lY_l)^0$ instead of the usual $Y_l\cdot Y_l=(-)^l[l]^{1/2}(Y_lY_l)^0$ but $J\cdot J=-\sqrt{3}(JJ)^0$ and $T\cdot T=-\sqrt{3}(TT)^0$ always, since $J\rightarrow iJ$ makes no sense. Still, positive definite zero coupling for tensors of integer rank could be obtained with the change $\langle lml-m|00\rangle=(-)^{l-m}[l]^{-1/2}$ to $(-)^m[l]^{-1/2}$. For half integer rank, no convention will ensure that zero coupling is always definite positive.

2. Normal and multipole representations

The two crucial equalities relating the zero coupled operators in terms of which the potential part of the Hamitonian, V, can be written are

$$-[X^{\dagger}_{\Gamma}(rs)X_{\Gamma}(tu)]^0=-(-)^{u+t-\Gamma}\left[\frac{\Gamma}{r}\right]^{1/2}\delta_{st}S^0_{ru}$$

$$+\sum_{\gamma}[\Gamma\gamma]^{1/2}(-)^{s+t-\gamma-\Gamma}\begin{Bmatrix}rs\Gamma\\ ut\gamma\end{Bmatrix}$$

$$\times(S^{\gamma}_{rt}S^{\gamma}_{su})^0\delta_{st}S^0_{ru} \tag{A16}$$

and its inverse

$$(S^{\gamma}_{rt}S^{\gamma}_{su})^0=(-)^{u-t+\gamma}\left[\frac{\gamma}{r}\right]^{1/2}\delta_{st}S^0_{ru}-\sum_{\Gamma}[\Gamma\gamma]^{1/2}$$

$$\times(-)^{s+t-\gamma-\Gamma}\begin{Bmatrix}r & s & \Gamma\\ u & t & \gamma\end{Bmatrix}[X^{\dagger}_{\Gamma}(rs)X_{\Gamma}(tu)]^0. \tag{A17}$$

In both cases the second term can be written through an elementary recoupling but the one body contractions need some care.

The potential energy appears naturally in terms of scalar products of the *normalized* creation operator $Z^{\dagger}_{rs\Gamma\Gamma_z}=(1+\delta_{rs})^{-1/2}X^{\dagger}_{rs\Gamma\Gamma_z}$, and its Hermitian conjugate $Z_{rs\Gamma\Gamma_z}$:

$$V=\sum_{\substack{r\leqslant s\\ t\leqslant u,(\Gamma)}} V^{\Gamma}_{rstu}Z^{\dagger}_{rs\Gamma}\cdot Z_{tu\Gamma}\equiv \sum_{\substack{r\leqslant s\\ t\leqslant u,(\Gamma)}} V^{\Gamma}_{rstu}\sum_{\Gamma_z} Z^{\dagger}_{rs\Gamma\Gamma_z}Z_{tu\Gamma\Gamma_z}, \tag{A18a}$$

$$V^{\Gamma}_{turs}=V^{\Gamma}_{rstu}=-(-)^{r+s-\Gamma}V_{srtu}=(-)^{r+s+t+u}V^{\Gamma}_{srut} =-(-)^{t+u-\Gamma}V^{\Gamma}_{rsut}. \tag{A18b}$$

In recoupling it is convenient to allow for complete flexibility in the summations over orbits, and we adopt the following convention

$$\xi_{rs}=(1+\delta_{rs})^{-1/2} \quad \text{if } r\leqslant s,$$

$$\xi_{rs}=\frac{(1+\delta_{rs})^{1/2}}{2} \quad \text{if no restriction,} \tag{A19}$$

so that the sums could be interpreted as restricted or not restricted. We write therefore

$$V=\sum_{\substack{r\leqslant s\\ t\leqslant u,\Gamma}} V^{\Gamma}_{rstu}Z^{\dagger}_{rs\Gamma}\cdot Z_{tu\Gamma} =-\sum_{(rstu)\Gamma}\xi_{rs}\xi_{tu}[\Gamma]^{1/2}V^{\Gamma}_{rstu}(X^{\dagger}_{rs\Gamma}X_{tu\Gamma})^0. \tag{A20}$$

Note that $\Sigma_{(rstu)}$ means that that we are summing as dictated by the values of ξ_{rs} and ξ_{tu}.

According to Eq. (A16), V can be transformed into

$$V=\sum_{(rstu)\gamma}\xi_{rs}\xi_{tu}[[\gamma]^{1/2}\omega^{\gamma}_{rtsu}(S^{\gamma}_{rt}S^{\gamma}_{su})^0 +\delta_{st}\hat{\delta}_{ru}[s]^{1/2}\omega^{0}_{russ}S^{0}_{ru}], \tag{A21}$$

where

$$\omega^{\gamma}_{rtsu}=\sum_{(\Gamma)}(-)^{s+t-\gamma-\Gamma}\begin{Bmatrix} r & s & \Gamma\\ u & t & \gamma\end{Bmatrix}V^{\Gamma}_{rstu}[\Gamma], \tag{A22a}$$

$$V^{\Gamma}_{rstu}=\sum_{\gamma}(-)^{s+t-\gamma-\Gamma}\begin{Bmatrix} r & s & \Gamma\\ u & t & \gamma\end{Bmatrix}\omega^{\gamma}_{rtsu}[\gamma]. \tag{A22b}$$

(We use $\Sigma_{(\Gamma)}$ to indicate that we sum over Pauli allowed Γ.) Equation (A17) suggests an alternative to Eq. (A21):

$$V=\sum_{(rstu)\gamma}\xi_{rs}\xi_{tu}[\gamma]^{1/2}\omega^{\gamma}_{rstu}\Big[(S^{\gamma}_{rt}S^{\gamma}_{su})^0 -(-)^{\gamma+r-s}\left[\frac{\gamma}{r}\right]^{1/2}\delta_{st}\hat{\delta}_{ru}S^{0}_{ru}\Big], \tag{A23}$$

where each term is associated with a two-body operator. The obvious check that Eq. (A23) is indeed Eq. (A21) comes from

$$-\sum_{\gamma}[\gamma]^{1/2}\omega^{\gamma}_{rstu}(-)^{\gamma+r-s}\left[\frac{\gamma}{r}\right]^{1/2}=[s]^{1/2}\omega^{0}_{russ}. \tag{A24}$$

The proof is left as an exercise [use Eq. (A22a) and Racah sum rule (A39)].

In a jt representation, by introducing explicitly the isospin in $\Gamma=JT,\gamma=\lambda\tau,r=j_r\,\frac{1}{2}$ etc., and the 6 j values

$$\begin{Bmatrix} 1/2 & 1/2T\\ 1/2 & 1/2\tau\end{Bmatrix}=\begin{array}{ccccc} T\tau & 00 & 01 & 10 & 11\\ & -1/2 & 1/2 & 1/2 & 1/6,\end{array} \tag{A25}$$

we find

$$\omega^{\lambda 0}_{rtsu}=\frac{1}{2}\sum_{(J)}(-)^{j_s+j_t-\lambda-J}\begin{Bmatrix} j_r & j_s & J\\ j_u & j_t & \lambda\end{Bmatrix}[J](V^{J0}_{rstu}+3V^{J1}_{rstu}), \tag{A26a}$$

$$\omega^{\lambda 1}_{rtsu}=\frac{1}{2}\sum_{(J)}(-)^{j_s+j_t-\lambda-J}\begin{Bmatrix} j_r & j_s & J\\ j_u & j_t & \lambda\end{Bmatrix}[J](V^{J0}_{rstu}-V^{J1}_{rstu}), \tag{A26b}$$

and reciprocally

$$V^{J0}_{rstu}=\frac{1}{2}\sum_{\lambda}(-)^{j_s+j_t-\lambda-J}\begin{Bmatrix} j_r & j_s & J\\ j_u & j_t & \lambda\end{Bmatrix}[\lambda](\omega^{\lambda 0}_{rtsu}+3\omega^{\lambda 1}_{rtsu}), \tag{A27a}$$

$$V^{J1}_{rstu}=\frac{1}{2}\sum_{\lambda}(-)^{j_s+j_t-\lambda-J}\begin{Bmatrix} j_r & j_s & J\\ j_u & j_t & \lambda\end{Bmatrix}[\lambda](\omega^{\lambda 0}_{rtsu}-\omega^{\lambda 1}_{rtsu}). \tag{A27b}$$

When the Hamiltonian is written as in Eq. (A20) we speak of the normal or V representation, and refer to the forms (A21) or (A23) as multipole, or ω representation. The latter is often called ph representation in the literature, because Eq. (A21) can be cast as a ph or Pandya-Talmi transformation by simply replacing the A_s and B_t operators by their ph transforms.

It is useful to have at hand the relationship between matrix elements in the jt and the j schemes. A single shell r in the former becomes a pair r_n and r_p in the latter

$$V^J_{r_n s_p t_n u_p} = \frac{(1+\delta_{rs})^{1/2}(1+\delta_{tu})^{1/2}}{2}(V^{J1}_{rstu} + V^{J0}_{rstu}),$$

$$V^J_{r_n s_p u_p t_n} = \frac{(1+\delta_{rs})^{1/2}(1+\delta_{tu})^{1/2}}{2}(V^{J1}_{rsut} - V^{J0}_{rsut}),$$

$$V^J_{r_n s_n t_n u_n} = V^J_{r_p s_p t_p u_p} = V^{J1}_{rstu}. \tag{A28}$$

3. Reduced matrix elements for l, σ, rY_1, and q operators

Conventions: r is the coordinate in units of the oscillator length $\sqrt{(\hbar/M\omega)}$. Radial wave functions are positive near the origin.

$\hat{j} = \hat{l} + \hat{s}$ (not $\hat{s} + \hat{l}$). The carets indicate operators.

Condon and Shortley phases for Y_{lm}.

(A) $\hat{\sigma} = 2\hat{s}$ and $\hat{l}$ matrix elements:

$$j' = l + 1/2, \quad j = l - 1/2,$$

$$f(j) = [j(j+1)(2j+1)]^{1/2},$$

$$\langle j' \| \hat{\sigma} \| j' \rangle = f(j')/j', \quad \langle j \| \hat{\sigma} \| j \rangle = -f(j)/(j+1),$$

$$\langle j' \| \hat{l} \| j' \rangle = l f(j')/j', \quad \langle j \| \hat{l} \| j \rangle = (l+1) f(j)/(j+1),$$

$$\langle j \| \hat{s} \| j' \rangle = \langle j' \| \hat{l} \| j \rangle = \left[\frac{2l(l+1)}{2l+1}\right]^{1/2}$$
$$= -\langle j' \| \hat{s} \| j \rangle = -\langle j \| \hat{l} \| j' \rangle. \tag{A29}$$

(B) $r^l Y_l$ matrix elements:

$$Y_l = \left(\frac{2l+1}{4\pi}\right)^{1/2} C_l,$$

$$\langle plj \| r^\lambda C_\lambda \| p' l' j' \rangle = \langle pl | r^\lambda | p' l' \rangle (-)^{j' - \lambda - 1/2} [jj']^{1/2} \times \begin{pmatrix} j & j' & \lambda \\ 1/2 & -1/2 & 0 \end{pmatrix}. \tag{A30}$$

(B1) r^1 and $r^1 Y_1$ matrix elements:

$$\langle pl | r | p+1\, l+1 \rangle = \sqrt{\frac{1}{2}(p+l+3)},$$

$$\langle pl | r | p+1\, l-1 \rangle = -\sqrt{\frac{1}{2}(p-l+2)}, \tag{A31}$$

$$\langle plj \| rC_1 \| p+1\, l+1\, j+1 \rangle = -\sqrt{\frac{p+l+3}{2}}\left[\frac{(2j+1)(2j+3)}{2(2j+2)}\right]^{1/2},$$

$$\langle plj \| rC_1 \| p+1\, l+1\, j \rangle = -\sqrt{\frac{p+l+3}{2}}\left[\frac{2j+1}{2j(2j+2)}\right]^{1/2},$$

$$\langle plj \| rC_1 \| p+1\, l-1\, j \rangle = \sqrt{\frac{p-l+2}{2}}\left[\frac{2j+1}{2j(2j+2)}\right]^{1/2},$$

$$\langle plj \| rC_1 \| p+1\, l-1\, j-1 \rangle = -\sqrt{\frac{p-l+2}{2}}\left[\frac{(2j-1)(2j+1)}{4j}\right]^{1/2}. \tag{A32}$$

(B2) r^2 and $r^2 Y_2$ matrix elements ($q_{0\hbar\omega}$ only for the latter):

$$\langle pl | r^2 | pl \rangle = p + 3/2,$$

$$\langle pl | r^2 | pl+2 \rangle = -[(p-l)(p+l+3)]^{1/2},$$

$$\langle pl | r^2 | p+2\, l \rangle = -\frac{1}{2}[(p-l+2)(p+l+3)]^{1/2},$$

$$\langle pl | r^2 | p+2\, l+2 \rangle = \frac{1}{2}[(p+l+5)(p+l+3)]^{1/2},$$

$$\langle pl | r^2 | p+2\, l-2 \rangle = \frac{1}{2}[(p-l+5)(p-l+4)]^{1/2}, \tag{A33}$$

$$\langle jl \| r^2 C_2 \| jl \rangle = -\frac{p+3/2}{2}\left[\frac{(2j+1)(2j-1)(2j+3)}{2j(2j+2)}\right]^{1/2},$$

$$\langle jl \| r^2 C_2 \| j+1\, l \rangle = (p+3/2)\left[\frac{3}{2}\frac{(2j+1)(2j+3)}{2j(2j+2)(2j+4)}\right]^{1/2},$$

$$\langle jl \| r^2 C_2 \| j+1\, l+2 \rangle = -\left[\frac{3}{2}\frac{(p-l)(p+l+3)(2j+1)(2j+3)}{2j(2j+2)(2j+4)}\right]^{1/2},$$

$$\langle jl \| r^2 C_2 \| j+2\, l+2 \rangle = -\left[\frac{3}{8}\frac{(p-l)(p+l+3)(2j+5)(2j+3)(2j+1)}{(2j+4)(2j+2)}\right]^{1/2}. \tag{A34}$$

Useful formulas involving $3j$ and $6j$ symbols:

$$\langle jmj'm' | JM \rangle = (-)^{j-j'+M}[J]^{1/2}\begin{pmatrix} j & j' & J \\ m & m' & -M \end{pmatrix}$$
$$= (-)^{j+j'-J}\langle j'm'jm | JM \rangle$$
$$= (-)^{j+j'-J}\langle j-mj'-m' | J-M \rangle, \tag{A35}$$

$$\begin{pmatrix} j & j' & J \\ m & m' & -M \end{pmatrix} = (-)^{j+j'+J}\begin{pmatrix} j' & j & J \\ m' & m & -M \end{pmatrix}$$
$$= (-)^{j+j'+J}\begin{pmatrix} j & j' & J \\ -m & -m' & M \end{pmatrix}. \tag{A36}$$

The $3j$ symbol is invariant under cyclical permutations

$$\langle jmj-m|00\rangle=[j]^{-1/2}(-)^{j-m}, \tag{A37}$$

$$\sum_J (-)^J[J]\begin{Bmatrix} j & j' & J \\ j' & j & k \end{Bmatrix}=(-)^{j+j'}[jj']^{1/2}\delta_{k0}, \tag{A38}$$

$$\sum_J [J]\begin{Bmatrix} j & j' & J \\ j & j' & k \end{Bmatrix}=1, \tag{A39}$$

$$\begin{Bmatrix} j & j & 0 \\ j' & j' & k \end{Bmatrix}=(-)^{j+j'+k}[jj']^{-1/2}. \tag{A40}$$

The $6j$ symbol is invariant under permutations of columns and under interchange of upper and lower indices in two columns.

APPENDIX B

1. 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 nontrivial properties.

a. Direct properties

(i) The $f^{\lambda\tau}$ matrix has twice as many elements as the W^{JT} matrix with $J=\lambda$.

If $r\neq s$ and $t\neq u$, W^{Γ}_{rstu} goes into ω^{γ}_{rtsu} and ω^{γ}_{rust} and the allowed values of Γ and γ are the same.

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

(ii) In the e representation we can write

$$H=\frac{1}{2}\sum_{\substack{r\leqslant t\\ s\leqslant u\,\gamma}}[\gamma]^{1/2}[(f^{\gamma}_{rtsu}+(-)^{s-u}f^{\gamma}_{rtus})(\mathcal{S}^{\gamma}_{rt}\mathcal{S}^{\gamma}_{su})^0 +(f^{\gamma}_{rtsu}-(-)^{s-u}f^{\gamma}_{rtus})(\mathcal{A}^{\gamma}_{rt}\mathcal{A}^{\gamma}_{su})^0] \tag{B1}$$

in terms of the $\mathcal{S}$ and $\mathcal{A}$ operators defined in Eq. (A14) . In the preceding example it means that out of eight possible $\gamma=2\tau$ combinations three are of $\mathcal{A}$ type and five of $\mathcal{S}$ type. Note that the matrices are always symmetric but the eigenvectors are linear combinations that are either of $\mathcal{S}$ or $\mathcal{A}$ type.

(iii) The trace of the f matrix *always* vanishes, as seen from

$$\sum_{\gamma,rt} f^{\gamma}_{rtrt}[\gamma]=\sum_{rt} P_{rr}P_{tt}\sum_{\gamma[\Gamma]}(-)^{r+t-\gamma-\Gamma}\begin{Bmatrix} r & r & \Gamma \\ t & t & \gamma \end{Bmatrix}W^{\Gamma}_{rrtt} =\sum_{rt}\frac{P_{rr}P_{tt}}{[rt]^{1/2}}W^{00}_{rrtt}=0, \tag{B2}$$

where we have used (2.1c) and sum rule (A10) from [1]. The matrix element W^{00}_{rrtt} is always zero because it is Pauli forbidden.

(iv) The variance of the f matrix is $\sigma^2_f=[(D-1)/8D]\sigma^2_W$ where σ^2_W is the variance of the W matrix. The calculation is better conducted in the m scheme:

$$H(W)=\sum W_{xx'}Z^{\dagger}_x Z_{x'},$$

$$x\equiv(ij),\quad x=1\cdots D^{(2)}/2,\quad i<j, \tag{B3}$$

$$H(f)=\sum f_{aa'}S_aS_{a'},$$

$$a\equiv(ij),\quad x=1\cdots D^2(ij \text{ unrestricted}). \tag{B4}$$

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

$$\sigma^2_W=\left(\frac{D^{(2)}}{2}\right)^{-1}\sum W^2_{xx'}, \tag{B5}$$

$$\sigma^2_f=D^{-2}\sum f^2_{aa'}=D^{-2}\sum 4\left(\frac{W_{xx'}}{4}\right)^2=\frac{D-1}{8D}\sigma^2_W. \tag{B6}$$

b. Asymmetric factorizations

Quadrupole renormalizations are mediated by terms of the form $k(\overline{q^{\prime}_p}\cdot\overline{q^{\prime}_{2\hbar\omega}}+\overline{q^{\prime}_{2\hbar\omega}}\cdot\overline{q_p})$. It is perhaps surprising that Eq. (2.3b) could produce such a result. In fact, it does it indirectly. What happens is that, for the particular type of matrices involved, two contributions with eigenvalues of same magnitude and opposite signs are present. It is by summing them that asymmetric factorizations appear. Let us see how, by studying $I\times I$ matrices f, whose nonzero 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. (2.2b) to this situation we have

$$\sum_x f_{ax}u_{xk}=u_{ak}e_k,\quad \sum_a f_{xa}u_{ak}=u_{xk}e_k. \tag{B7}$$

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

$$|k\rangle=\sum_{i=1,I}u_{ik}|i\rangle=\sum_{a=1,K}u_{ak}|a\rangle+\sum_{x=K+1,I}u_{xk}|x\rangle. \tag{B8}$$

By reversing simultaneously the sign of e_k and u_{xk} ($e_k\rightarrow-e_k$, $u_{xk}\rightarrow-u_{xk}$, $\forall x$) Eq. (B7) remains unchanged telling us that

$$|\overline{k}\rangle=\sum_a u_{ak}|a\rangle-\sum_x u_{xk}|x\rangle \tag{B9}$$

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

$$\sum_i u_{ik}u_{ik'}=\sum_a u_{ak}u_{ak'}+\sum_x u_{xk}u_{xk'}=\delta_{kk'} \tag{B10}$$

and taking overlaps

$$\langle k|\overline{k'}\rangle=\sum_a u_{ak}u_{ak'}-\sum u_{xk}u_{xk'}=0, \tag{B11}$$

leading to

$$\sum_a u_{ak}u_{ak'}=\sum_x u_{xk}u_{xk'}=\frac{1}{2}\delta_{kk'}. \tag{B12}$$

From these results we may construct the spectrum of f. Let us call $M=\min(L,K)$. We have: M positive eigenvalues e_k $(k=1,M)$, M negative ones $e_{\overline{k}}=-e_k$ $(\overline{k}=M+k)$, 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

$$\sum (f_{xa}-g_a g_x)^2=\min. \tag{B13}$$

Variation with respect to f_x and f_a leads to

$$\sum_x f_{xa}g_x=g_a\sum_x f_x^2, \quad \sum_a f_{xa}g_a=g_x\sum g_a^2, \tag{B14}$$

and given that (B13) is invariant under $g_x\to\sigma g_x$ $g_a\to\sigma^{-1}g_a$ we may request

$$\sum_x g_x^2=\sum_a g_a^2=e \tag{B15}$$

and Eq. (B14) becomes Eq. (B7) 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 C

1. Baranger and Kumar revisited

In two important papers Baranger and Kumar attempted to derive from a realistic interaction the pairing plus quadrupole forces adapted to a space of two major shells [1] 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 [35].

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 [1,35]

$$H_P=-G_x(P_p^\dagger+P_{p+1}^\dagger)\cdot(P_p+P_{p+1}), \tag{C1}$$

$$H_q=-\frac{\chi'}{2}(q_p+q_{p+1})\cdot(q_p+q_{p+1}), \tag{C2}$$

with the normalized versions in Eqs. (2.9) and (2.10), which we write explicitly by borrowing numbers from Table II and remembering that $\hbar\omega_0=9$ MeV:

$$H_{\overline{P}}=-0.32\hbar\omega\left(\frac{P_p^\dagger}{\sqrt{\Omega_p}}+\frac{P_{p+1}^\dagger}{\sqrt{\Omega_{p+1}}}\right)\left(\frac{P_p}{\sqrt{\Omega_p}}+\frac{P_{p+1}}{\sqrt{\Omega_{p+1}}}\right),$$
$$H_{\overline{q}}=-0.216\hbar\omega\left(\frac{q_p}{\mathcal{N}_p}+\frac{q_{p+1}}{\mathcal{N}_{p+1}}\right)\left(\frac{q_p}{\mathcal{N}_p}+\frac{q_{p+1}}{\mathcal{N}_{p+1}}\right). \tag{C3}$$

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

$$\frac{1}{\sqrt{2}}\left\langle\frac{q_p}{\mathcal{N}_p}+\frac{q_{p+1}}{\mathcal{N}_{p+1}}\middle|\frac{q_p+q_{p+1}}{\sqrt{\mathcal{N}_p^2+\mathcal{N}_{p+1}^2}}\right\rangle$$
$$=\frac{1}{\sqrt{2}}\frac{\mathcal{N}_p+\mathcal{N}_{p+1}}{\sqrt{\mathcal{N}_p^2+\mathcal{N}_{p+1}^2}}=0.98 \text{ for } p=3 \tag{C4}$$

seems large enough to identify $H_{\overline{q}}$ and H_q to a good approximation. Of course there is some risk because in the norms defined in the vector space of the multipole representation the S_{rt} operators are *all* treated as unit vectors. In a midshell situation, as in ^{28}Si, the $p+1$—upper—shell is very poorly represented in the wave functions. Then the large overlap is meaningless.

With this proviso in mind we equate the traditional and the new forms. Recalling that $\hbar\omega=40\,A^{-1/3}$ [20], and writing the norms in terms of $A_{\rm mp}$ as in Eqs. (2.4) and (2.5) we find for one shell

$$\frac{0.216\hbar\omega}{\mathcal{N}_p^2}\cong\frac{1}{2}\,\frac{216}{A^{1/3}A_{mp}^{4/3}}=\frac{\chi'}{2}\equiv\frac{\chi_0'}{2}A^{-5/3},$$
$$\frac{0.32\hbar\omega}{\Omega_p}\cong\frac{19.51}{A^{1/3}A_{mp}^{2/3}}=G\equiv G_0A^{-1}, \tag{C5}$$

and for two shells,

$$\frac{0.216(2\hbar\omega)}{\mathcal{N}_p^2+\mathcal{N}_{p+1}^2}\cong\frac{1}{2}\,\frac{216}{A^{1/3}A_{c'p}^{4/3}}=\frac{\chi'}{2}\equiv\frac{\chi_0'}{2}A^{-5/3},$$
$$\frac{0.32(2\hbar\omega)}{\Omega_p+\Omega_{p+1}}\cong\frac{19.51}{A^{1/3}A_{c''p}^{2/3}}=G\equiv G_0A^{-1}, \tag{C6}$$

where we have expressed the averaged norms in terms of $A_{c'p}$ 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^{-1}. It is possible to understand their origin: They amount to setting $A_{mp}=A$, which makes sense in comparing strengths in distant regions, but is locally wrong. If taken at face value, the $A^{-5/3}$ local behavior predicts variations in the moments of inertia of neighboring that are much larger than the observed ones [36,37].

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

$$(A_{mp}/A_{cp})^{k/3}=\left(\frac{2p+3}{2p+4}\right)^{k}, \tag{C7}$$

with $k=4$ for χ' and $k=2$ for G. If our identifications were correct, these discrepancies should not exist, and they are related to the risk we described after Eq. (C4): There is no guarantee that we can approximate well the operator q_p+q_{p+1} by q_p+q_{p+1}. The compromise χ' in Eq. (C6) 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 wave functions, then the large overlap in Eq. (C4) 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 obtained $\chi'_0=203$ (vs our 216) for one shell, but for two shells the value was reduced by a factor of about 0.6 at $p=2$, close to $(7/8)^4$ calculated in Eq. (C7). When faced with this unwanted reduction, instead of blaming the $q\cdot q$ form, they declared incorrect their method of extraction which—under a primitive guise—is identical to ours and correct to within some details (discussed in Sec. III B). Then, to obtain the coupling constant, they proceeded to invent another method, unrelated to any interaction (see *Note 2* below).

At this point Ref. [1] 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 showing what the scaling must be.

Now observe carefully Eqs. (C5) and (C6) to discover the detail that repairs the damage. The only sensible way to define χ'_0 for one shell is to ''equate'' $A_{mp}\approx A$, while for two shells we must take $A_{cp}\approx A$ and now χ'_0 is identical to 216 in both cases.

There is no contradiction between χ'(1 shell)$\neq\chi'$(2 shells) at a given nucleus and χ'_0(1 shell)$=\chi'_0$ (2 shells), both calculated in different nuclei.

The point is rather subtle and 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 [35] is approximately centered at the oscillator closures $Z=70$ and $N=112$, which meets this restriction, and that the parameters used were (in MeV):

$$\chi'_0\approx 280,\ \ G_{0\pi}=27,\ \ G_{0\nu}=22,$$

somewhat larger than those in Eq. (C6) but quite consistent with the renormalized values of Sec. IV. [The need to use different G_0 values for neutrons and protons is readily explained by (C6). 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. (C6) is generalized to M major shells. It is elementary to prove that $\chi'=O(A^{-1/3}M^{-4})$, and that the overlap tends to $\sqrt{5/9}$. It means that to simulate—never mind how remotely—the behavior of its realistic counterpart, the conventional $q\cdot q$ force must be affected by a vanishingly small χ'.

Note 2: on the second method of extraction in [1]. To replace direct extraction of χ' 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 but assumes very specifically that particles move in two major shells. Hence the presence of two terms in the denominator of the resulting estimate:

$$\chi'=\frac{\hbar\omega}{\mathcal{N}_p^2+\mathcal{N}_{p+1}^2}$$

[Eqs. (72) and (73) and the paragraph following them in [1], but here we have introduced the norms instead of their asymptotic values]. This is the same χ' of Eq. (C6), except that a factor 4×0.216 has been set to unity.

The critical dependence on the number of shells that are taken to be active makes the result suspect. However, it may also mean that it is a profound one since two shells seem to be the natural valence space to describe rotational motion. (See [22].) It should be noted that the value of χ' deduced by Mottelson in [27] is exactly half of the Baranger and Kumar one [1].

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