Nuclear Characteristics and Empirical Mass Sum Rules*

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(Received 17 November 1971)

The Garvey-Kelson mass sum rule is known to be violated when $Z=N=$odd, $Z=N+1=$even, or $Z=N+1=$odd nuclei are considered. This violation is a result of the lack of cancellation of certain two-body matrix elements. These matrix elements can be calculated assuming various models of the nuclei involved, e.g., deformation, level ordering, etc., and the amount by which the sum rule is violated empirically can then be used to distinguish the most appropriate model. The results of this empirical determination of nuclear characteristics agree quite well with the results of more involved calculations and conform to the generally accepted picture of nuclei in the s-d shell.

I. INTRODUCTION

Since the nucleus is a complex system of protons and neutrons interacting via complicated potentials, it is not surprising that the concept of what the wave function is for a nucleus is far from simple. Calculations which assume simple, determinantal wave functions and utilize realistic interactions have had little success,[1] and attention has turned from such Hartree-Fock (HF) methods to more complicated techniques such as Brueckner-Hartree-Fock or HF with perturbation corrections.[2] In the latter case the wave function is a linear combination of a large number (in principle, infinity) of determinants with the amplitude of the original HF determinant rather small. If one chooses, instead, to retain the single-determinant description, one must employ an effective interaction which in some way will implicitly contain the correlation effects. The one-body part of the Hamiltonian will, in the same way, be modified so that the Hamiltonian under consideration assumes the form

$$H=\sum_i t_i+\sum_{i<j} v_{ij}\rightarrow\sum_i \bar{t}_i+\sum_{i<j}\bar{v}_{ij}\,, \tag{1}$$

where the bar indicates that the operator is "effective." The usual procedure then is to fit the parameters of the effective interaction, $\bar{v}$, via shell-model calculations of nuclear spectra, treating only the "valence" nucleons. With an effective interaction so determined, restricted HF calculations may be carried out in the same spirit. Together with projection of angular momentum this provides quite a good approximation to an exact diagonalization and can be extended to systems with many valence particles.[3] The success of such calculations indicates that, for some purposes, the use of single determinantal, intrinsic wave functions and effective interactions provides a convenient description of a nucleus.

Based on a simplified version of this model, a set of mass sum rules has been devised which are remarkably well satisfied. A brief description of the model and the sum rules is given in the next section.

II. MASS SUM RULES

If a HF calculation were carried out for an even-even, $N=Z$ nucleus, with a charge-symmetric potential, each single-particle level would be fourfold degenerate. Thus two protons and two neutrons, with angular momentum projections positive and negative, can be considered as occupying each level. If the Coulomb force were included or the nucleus under consideration did not have $N=Z=$even, then the HF potential would not be invariant under time reversal and isospin conjugation and the fourfold degeneracy would be removed. Such calculations have been performed and the degeneracy is in fact quite appreciably broken.[4] In the spirit of the effective interaction, however, it can still be assumed that the expectation values of the one-body operator in the occupied levels are unaffected by either this symmetry breaking or the addition of a small number of particles to the system. Then, following Garvey and Kelson (G-K),[5] if the nuclei shown schematically in Fig. 1 are considered, a simple mass sum rule can be inferred: Namely,

$$M(N+2, Z-2)-M(N, Z)+M(N, Z-1)-M(N+1, Z-2)$$
$$+M(N+1, Z)-M(N+2, Z-1)=0\,. \tag{2}$$

Such a set of six nuclei will henceforth be designated by the Z and N of the nucleus with the largest value of $Z-N$. When this nucleus has $Z=N$ = even, the case shown in Fig. 1, there is cancellation not only of the one-body contributions to the energy and the two-body interactions amongst particles in the same levels, but also amongst particles in different levels. In order to obtain this cancellation it was assumed that the single-particle wave functions vary slowly for neighboring nuclei.

This mass sum rule was tested for over six hundred sets of nuclei with the average deviation from zero being about 200 keV.[6] Furthermore, the deviations were randomly distributed around zero showing that there was no systematic error. These results are quite remarkable when one considers the actual wave functions of the nuclei being considered and all of the approximations made.

It is quite significant to point out that in the majority of the cases tested, those *not* characterized by $Z=N$ = even, the complete cancellation mentioned above does not occur. There is cancellation of the one-body contributions and the intralevel interactions, but not of the interlevel interactions. For example, in the case shown in Fig. 2 there is residual interaction of a neutron in level 2 with a proton in level 1, which enters with a positive sign, and one of a neutron in level 3 with a proton in level 1 entering with a negative sign. The success of the mass sum rules, in spite of this lack of cancellation, strongly indicates that the effective interaction contains a large Majorana component which emphasizes intralevel matrix elements. Indeed, for the typical effective interactions employed, the intralevel matrix elements are, on the average, about 3 times larger than interlevel matrix elements. It is also useful to note that the ratio of typical variations of these matrix elements, for various states, is also roughly 3 to 1. The deviations of empirical masses from the sum rule are consistent with the small variations of the interlevel matrix elements.

III. VIOLATIONS OF THE SUM RULE

The fact that the mass sum rules are so well satisfied in a way *reduces* their usefulness in extracting structural information from the data. The success of the mass sum rule indicates that there is, to a large extent, a cancellation of the large matrix elements, and remaining deviations, being differences of small numbers, are not amenable to model calculation.

There are, however, three cases for which the simple model does not predict cancellation of the intralevel interactions. These are the cases characterized by $Z=N$ (odd), $Z=N+1$ (even), and $Z=N+1$ (odd). The simple single-particle structures for these cases are shown in Fig. 3. For these cases the noncanceling interactions are given in Fig. 4. It is significant to note that in

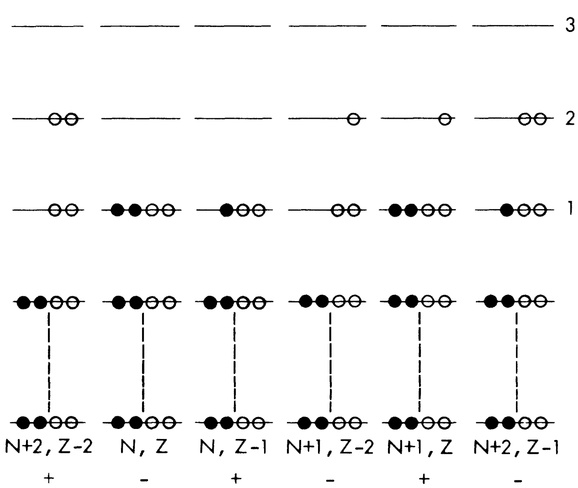

FIG. 1. Schematic representation of the single-particle levels of the six nuclei entering the G-K sum rule for $N=Z$ = even. The sum rule is obtained by taking a linear combination of these masses with alternating signs, as shown. Here the solid circles represent protons and the open circles neutrons.

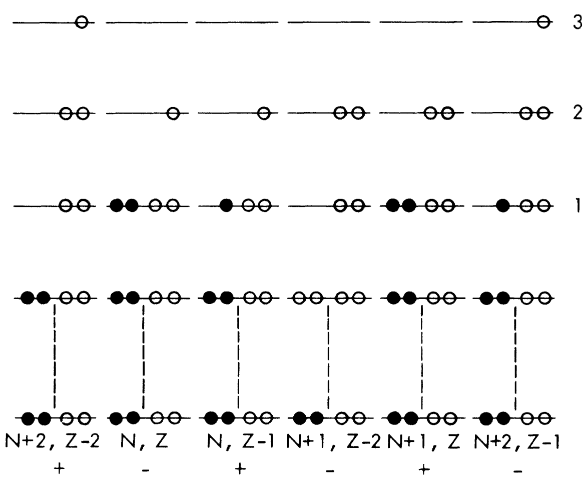

FIG. 2. Schematic representation of the single-particle levels of the six nuclei entering the G-K sum rule for the case $Z=N-1$ = even. This case is typical of the majority of those for which the sum rule is satisfied in that there is not complete cancellation of interlevel interactions. For example, the interaction of the neutron in level 3 and the proton in level 1, occurring in the last nucleus above, is not canceled by a corresponding interaction in another nucleus.

each case the deviation from the sum rule, Δ, is the difference between an interlevel and an intralevel interaction. When the mass sum rule is applied to these types of nuclei the violations are about 1–2 MeV, as compared with deviations of 200 keV, on the average, for other types of nuclei.

The amount by which the sum rules are violated for these cases and the matrix elements responsible for the violation form the basis of a method of determining some aspects of the structure of the nuclei being considered.

IV. PRESENT MODEL

The basic idea of the present calculation is to take seriously the simple single-particle picture. Since the observed deviations for the three cases described above are large, a calculation of them should be relatively insensitive to the details of the model employed. Thus, using a standard effective two-body interaction, the noncanceling matrix elements are calculated under various

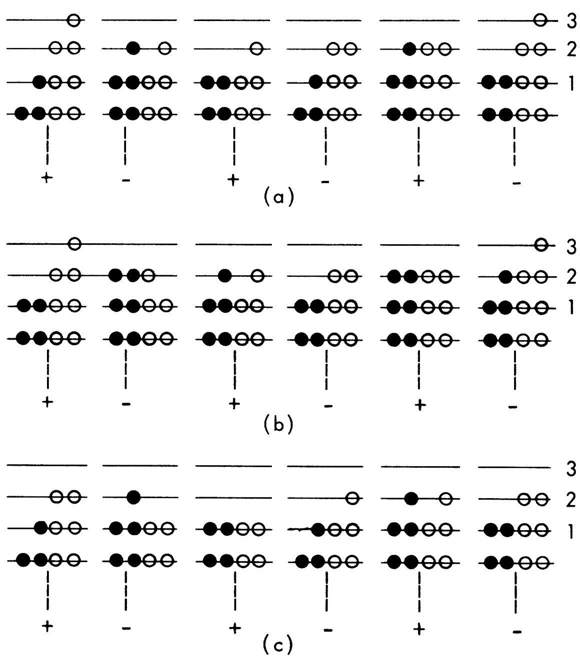

FIG. 3. Schematic representation of the single-particle levels of the six nuclei entering the G-K sum rule for the cases (a) $N = Z$ (odd), (b) $Z = N+1$ (even), and (c) $Z = N+1$ (odd). For these cases the sum rules should be violated. For example in case (a), in the level labeled (2), there is a p-n interaction in the fifth nucleus which is not canceled by the same interaction in any other nucleus. A similar lack of cancellation of interactions within a given level occurs in cases (b) and (c). Instead there is also an uncanceled interaction between nucleons in different levels in each of these cases.

assumptions about deformation and level ordering, using wave functions which come from HF calculations. The Δ's can then be calculated and compared with the empirical values to determine which set of assumptions is consistent with the data.

Since attention will be focused primarily on s-d-shell nuclei, the force chosen was a Gaussian with the Rosenfeld exchange admixtures, i.e.,

$$V(r) = V_0 e^{-(r/\mu)^2}(W + MP_x - HP_\tau + BP_\sigma) \qquad (3)$$

with

$$W = -0.13, \quad M = 0.93,$$

$$H = -0.26, \quad B = 0.46,$$

$$V_0 = -55.75 \text{ MeV}, \quad \mu = 1.48 \text{ fm}$$

and with the harmonic-oscillator constant, $\alpha = (m\mu/h)^{1/2}$, chosen such that

$$\alpha\mu = 1.$$

The wave functions employed were taken from a HF calculation using a similar force wherein the O^{16} core was considered inert and the variational space was limited to the s-d shell.[7] Although this is a severe truncation, the wave functions are quite similar to those obtained in a full HF calculation in a very large space employing a realistic potential.

The resultant Δ's are, of course, dependent on the particular force and wave functions employed, but this sensitivity is of the order of a few hun-

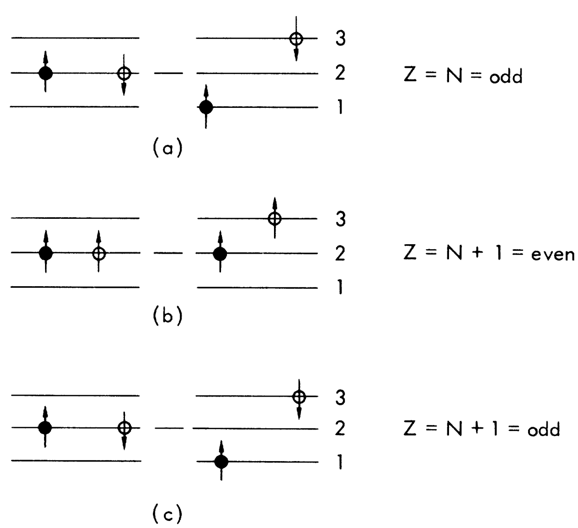

FIG. 4. The noncanceling matrix elements responsible for the violation of the G-K sum rules. These differences, denoted by Δ in the text, represent the amount by which the sum rule should be violated for the three cases (a) $N = Z$ (odd), (b) $Z = N+1$ (even), and (c) $Z = N+1$ (odd).

dred keV for reasonable forces and for wave functions of the same sign but differing size and deformation. Fortunately the quantities of interest are an order of magnitude larger than these variations.

V. RESULTS AND CONCLUSIONS

The results of the calculation are summarized in Table I, and are best presented by describing this table. Column 1 gives the "anchor" nucleus of the mass sum rule, namely, that nucleus of the sextet which has the largest proton excess, $Z-N$. Thus, it is according to the proton and neutron numbers of this particular nucleus that the three cases ($Z=N=\text{odd}$, $Z=N+1=\text{even}$, $Z=N+1=\text{odd}$) are classified. As was shown above, each of these three cases involves a p-n interaction where the interacting particles are in the same level.

The identity of this "active" level is shown in column 2, where the six fourfold-degenerate single-particle levels of the s-d shell are odd numbered from 9 to 19. (This corresponds, for example, to the Z of a nucleus which has all lower proton levels filled plus a single proton in the level in question.)

Once the model nuclear interaction has been chosen, the calculated Δ's depend only on the structure and composition of the single-particle states, and these, in turn, primarily depend on the nuclear deformation. Throughout the table and the accompanying text the three possible axially symmetric deformations, spherical, prolate, and oblate, are designated by S, P, and O and a nonaxially symmetric deformation is designated by N.

There are preliminary indications as to which deformation should be used in each case. The first one, essentially experimental, is based on the systematics of ground-state spins, and is summarized in column 3 of the table. The underlying assumption is that the ground-state spin of an even-odd nucleus is determined solely by the odd nucleon. If the single-particle states are characterized by the projection of angular momentum along a body axis of symmetry, then the total angular momentum will equal that projection. For odd-odd nuclei, it is further assumed that ground-state spin will be equal to the sum of the two odd particles' projected angular momenta. These assumptions are consistent with the properties of the interactions, and with the behavior of the wave functions under angular momenta projection. They basically state that if a nucleus is associated with an intrinsic state which is axially

TABLE I. Predicted deformations. Columns 3, 4, and 10 contain the predicted deformations based on spin systematics, Hartree-Fock calculations, and mass sum-rule violations Δ, respectively. S, P, and O refer to the three possible axially symmetric shapes, while N indicates a nonaxially symmetric deformation. The "anchor" nucleus is given in column 1 and the active level is labeled in column 2 (see Sec. V). Column 5 contains the empirical values of Δ, and columns 6–9 (SPON) the calculated values obtained employing the various possible deformations.

"Anchor" nucleus	Active level	Deformation: Spin systematics	Deformation: Hartree-Fock	Deviation from mass sum rule, Δ: Empirical (MeV)	Calculated: S (MeV)	Calculated: P (MeV)	Calculated: O (MeV)	Calculated: N (MeV)	Deformation Mass sum-rule violations Δ
F^{17}	9	P	P	2.8	0.1	3.2	1.4	0.8	P
F^{18}	9	P	P	1.9	0.5	1.6	0.8	1.1	P
N^{19}	9	P	P	3.8	0.0	3.5	1.4	1.0	P
Na^{21}	11	P	P	2.1	0.8	1.7	1.0	0.6	P
Na^{22}	11	P	N	2.0	0.1	0.9	−0.1	1.9	N
Mg^{23}	11	P	N	2.3	0.7	1.0	0.3	2.1	N
Al^{25}	12	P	N	1.9	2.2	2.3	2.1	2.2	All
Al^{26}	13	P	P (N)	1.9	−0.4	−0.9	0.0	−0.1	None
Si^{27}	13	P	P	2.8	2.6	2.7	3.4	1.3	P
P^{29}	15	O	O	1.7	2.8	1.8	1.5	0.7	O (P)
P^{30}	15	O	O (N)	2.1	2.7	−0.6	1.8	0.2	O
S^{31}	15	O	N	1.5	3.6	0.7	−0.1	1.3	N
Cl^{33}	17	O	N	1.6	0.9	2.4	0.8	1.6	N
Cl^{34}	17	O	N	0.9	0.2	−1.6	−1.2	1.5	N
Ar^{35}	17	O	O	1.1	0.3	2.9	1.6	0.1	O
K^{37}	19	S	O (S)	1.7	1.5	3.0	0.5	0.3	S
K^{38}	19	S	S	0.9	1.3	2.4	1.6	1.7	S
Ca^{39}	19	S	S	1.3	0.8	3.7	2.9	2.9	S

symmetric and if the ground state is projectable from this intrinsic state, then the lowest state will be the one with minimal angular momentum. It must be emphasized, however, that unless one presupposes axial symmetry, no inference can be made regarding the sign of such deformations. Also, since each case involves six nuclei, a wholly consistent determination of an axial deformation is not always possible. The table, in such cases, indicates the most plausible assignment.

Since the axial symmetry, or lack of it, refers to the *intrinsic* state, which is only indirectly related to physical states and observables, one has to resort to theoretical considerations in order to differentiate between these two general categories of deformation (axial vs nonaxial). The theoretical determination is based on a HF calculation, and is summarized in column 4. Here, again, there is a certain ambiguity due to the participation of six nuclei in each mass sum rule.

The experimental values of Δ are given (in MeV) in column 5. The uncertainties in the masses are usually very small. In the case of Cl^{34}, which has a 0^+ $(T=1)$ ground state, the first excited 3^+ $(T=0)$ state at 140 keV has been used instead.

The theoretically calculated values of Δ are given in columns 6–9 (in MeV). All four numbers have been given, although one or two possibilities are actually ruled out in each case by experimental ground-state spin systematics. However, since such systematics do in fact involve various assumptions, it was felt that the calculation of Δ should be regarded as a completely independent model test case.

In column 10 are listed the deformations indicated by the best fit of calculated to experimental Δ. It must be remembered, however, that this is not a deformation associated with one particular nucleus. Rather, because of the nature of the mass sum rule and the cancellation of interactions, it is an average "effective" deformation for the group of nuclei centered around the mass number of the "anchor" nucleus.

With the exception of one case, there is an overall consistency of assignments of deformation by the three methods: ground-state spin systematics (unable to differentiate nonaxial deformation), HF calculations, and mass sum rules. Keeping in mind that the model is based on extremely simple assumptions and that no parameter searches or numerical fittings were carried out, this consistency is indeed pleasing. One may therefore conclude that this semiempirical procedure provides a method for differentiating between axially symmetric and nonaxially symmetric intrinsic states.

Finally, a point should be emphasized which is often not clearly understood. Namely, intrinsic states are not actual states of the nuclear system. Their significance stems from the fact that they are related to certain *sets*, or groups of states. The most notable example is the deformed intrinsic state which is related to (in fact, is considered a linear combination of) the members of a rotational band in one nucleus. Here the intrinsic state and the intrinsic deformation have been related to a *set* of states, the ground states of six *different* nuclei, thereby imparting to this concept further meaning.

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*Work supported in part by a grant provided by the Research Council of Texas A&M University.

† Much of this work was performed while I. Kelson was a visitor at Texas A&M University under the auspices of the Research Council of Texas A&M University.

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