Semiempirical determination of effective p-n monopole matrix elements

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A method for extracting effective p-n monopole matrix elements from experimental data is developed and applied to nuclei just below ^{208}Pb. Eight effective monopole matrix elements are extracted from a fit to 38 experimental data with an overall rms deviation of 116 keV. The resulting matrix elements are compared with those from semirealistic effective interactions.

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I. INTRODUCTION

It is widely recognized that the valence p-n interaction is an essential key to the understanding of nuclear structure and its evolution with N and Z [1–5]. The effects of the p-n interaction appear most vividly in two more or less distinct empirical aspects, reflecting, respectively, its quadrupole and monopole components. The quadrupole component is primarily responsible for the development of collectivity in nuclei removed from closed shells. Indeed, this fact accounts for the success of the N_pN_n scheme [4] in correlating the nuclear data in shape-transitional regions leading to deformation. The monopole component is critical in shifting and determining the basic single-particle energies (spe's) of the underlying shell structure. This in turn determines the shell gaps and closures and hence the valence space in which the quadrupole component acts. The importance of the monopole component of the p-n interaction in eradicating the proton shell gap at Z=38 when $N \geq$60, leading to the virtually instantaneous onset of deformation in the Sr, Zr, and Mo isotopes, was discussed in Ref. [3]. Figure 1 [6] illustrates the effect of the monopole p-n interaction on the spe's of the N = 50–82 shell between ^{91}Zr (Z = 40) and ^{131}Sn (Z = 50). The principal change, a dramatic lowering of the $\nu(1g_{7/2})$ orbit, is largely due to the filling of the $\pi(1g_{9/2})$ orbit in this region, since these two orbits have a large overlap and thus a large attractive monopole interaction strength. Studies by Goodman [7], Heyde [5], and others [8, 9] have further elucidated the importance of this component of the effective nuclear force in several mass regions, and in doing so have also linked the concepts of shape coexistence and intruder states into a coherent picture.

Despite these widespread effects of the monopole p-n interaction, there is no acceptable model for its matrix elements. Semirealistic matrix elements, which success-

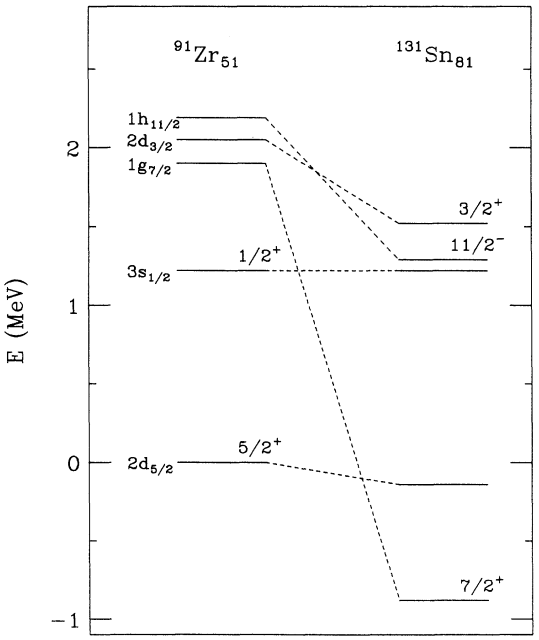

FIG. 1. Relative single-particle and single-hole energies, respectively, in ^{91}Zr and ^{131}Sn, showing their changes as a function of N and Z. The $d_{5/2}$ energy is set equal to zero in ^{91}Zr and the energies are further normalized so that the $s_{1/2}$ level has the same energy in the two nuclei. Based on Ref. [6].

fully describe many aspects of nuclear structure, are unable to reproduce spherical single-particle systematics in passing through a shell. As a consequence, many microscopic analyses simply ignore the problem, using a p-n force with no monopole component and choosing the spherical single-particle energies (in some way) for the nucleus under discussion [10, 11]. Monopole p-n effects can be included in a minimal way through the use of a linear interpolation procedure [12], but this ignores any specific dependence on the orbits that are filling. There has also been an attempt to parametrize the monopole matrix elements (mme's) in terms of the proton and neutron quantum numbers [13], but so far this has not been done systematically.

In this paper, we propose a systematic approach to extracting effective monopole p-n matrix elements from experimental data. Our approach is similar in spirit to that of Ref. [14], where effective p-n matrix elements for the light rare-earth region were obtained by a scaling procedure in the context of the spherical Hartree-Fock-Bogoliubov (HFB) method. However, it really owes its origin to the work of Arenas Peris and Federman [9] on intruder states. As in Ref. [9], we consider the p-n mme's as variational parameters, which are determined by fits to *appropriate* experimental data. However, as we will discuss in Sec. II, we have made some extensions and improvements of their method.

The basis of our proposed method is the observation that in nuclei in which at least one type of particle (neutron or proton) is fairly near a magic number, the generalized seniority scheme [15] should be applicable. In such cases, low-lying states should be dominated by configurations in which the neutrons and/or the protons have generalized seniority (w) zero. Whenever this is the case, the only component of the p-n interaction that contributes is the monopole. By judicious fits to the binding energies and spectra of such nuclei, we can hopefully extract the mme's of interest. In Sec. II, we describe the method and present some criteria for choosing the nuclei to which it should apply.

As a first application of our method, we have considered nuclei in the mass region just below ^{208}Pb. In Sec. III, we discuss the data that were included in the fits as well as the other required input and then describe our results. Finally, in Sec. IV, we discuss the principal conclusions of our work. A major thrust of our effort has been to clarify the practical issues that must be addressed before our method can be used systematically to extract p-n mme's. As we will see in the discussion to follow, a principal limitation concerns the lack of experimental data, which may hopefully be remedied in the future through newly available experimental opportunities.

II. THEORETICAL FRAMEWORK

Nuclei away from closed shells are dominated by two competing correlation structures. Pairing correlations, resulting from the interactions between identical nucleons, give rise to a spherical system with (to a good approximation) conserved generalized seniority. Neutron-proton correlations, resulting primarily from the quadrupole-quadrupole interaction, lead to a deformed system and break generalized seniority. The interplay of these two correlation structures is governed by the ratio $\frac{N_p N_n}{N_p+N_n}$, where N_p and N_n are the number of valence protons and neutrons (or holes), respectively. Empirical systematics suggest that when this ratio is less than ≈ 2, the system will be dominated by pairing correlations. If, furthermore, the system is either even-even or odd-mass, the structure of the lowest states will be dominated by configurations in which the neutrons and/or the protons have generalized seniority $w = 0$ and thus $J^\pi = 0^+$. For such states, the only component of the p-n interaction that is active is the monopole. This observation provides the basis of the theoretical framework we use to extract monopole p-n matrix elements from experimental data.

For systems of the type just described, the energies of the lowest states relative to that of the relevant doubly magic core can be expressed as (i denotes the state)

$$E_i = \langle H_n \rangle_i + \langle H_p \rangle_i + \langle V_{p\text{-}n} \rangle_i \ , \tag{1}$$

where

$$\langle V_{p\text{-}n} \rangle_i = \sum_{j_n j_p} n^n_{j_n}(i)\ n^p_{j_p}(i)\ \bar{V}^{p\text{-}n}_{j_p j_n} \ . \tag{2}$$

Here, H_ρ denotes the Hamiltonian for particles of type ρ (n or p), including both the single-particle energies and the identical-nucleon interaction. Also, $\bar{V}_{j_p j_n}$ represents the average or monopole matrix element between a proton in orbit j_p and a neutron in orbit j_n and $n^\rho_{j_\rho}(i)$ is the number of valence nucleons in orbit j_ρ in the state i.

The basic idea of our analysis will be to extract E_i and $\langle H_\rho \rangle_i$ from experimental data (combined with calculations, where necessary) and $n^\rho_{j_\rho}(i)$ from calculations. If this can be done reliably, the only remaining unknown quantities that determine the energies are the p-n mme's.

With this in mind, we set up a system of nonlinear equations (one for each state with the appropriate generalized-seniority structure) to determine (in a least-squares sense) the unknown mme's. The system of equations can be written compactly as

$$\sum_{j_p j_n} A^i_{j_p j_n} \bar{V}^{p-n}_{j_p j_n} = B^i \ , \tag{3}$$

where, as before, i specifies the nuclear state,

$$B^i = E_i - \langle H_p \rangle_i - \langle H_n \rangle_i \tag{4}$$

and

$$A^i_{j_p j_n} = n^p_{j_p}(i)\ n^n_{j_n}(i) \ . \tag{5}$$

This overcomplete system of equations, once set up, can be solved using standard iterative techniques.

The quantities E_i can be directly extracted from experimental data. A natural first thought is that, as in Ref. [9], $\langle H_p \rangle_i$ and $\langle H_n \rangle_i$ can also be obtained from experimental energy differences, but now between the doubly magic core and the semimagic nuclei with the correct numbers of valence nucleons. However, in a system with active neutrons and protons, such a procedure ig-

nores changes in the structure of the identical-particle wave functions that may be induced by the same p-n monopole interaction that we want to determine. Thus, in our calculations we modify these quantities so that they are consistent with the extracted mme's. Namely, at each step of the iteration procedure, we calculate the modifications to the bare single-particle energies $\epsilon^{\rho}_{j_\rho}$ that result from the monopole interaction with particles of the other type and then determine the changes in $\langle H_n \rangle_i$ and $\langle H_p \rangle_i$ that result. The *effective* single-particle energies $\tilde{\epsilon}^{\rho}_{j_\rho}$ are related to the bare values by [$\rho' = p(n)$ if $\rho = n(p)$]

$$\tilde{\epsilon}^{\rho}_{j_\rho} = \epsilon^{\rho}_{j_\rho} + \sum_{j_{\rho'}} n^{\rho'}_{j_{\rho'}} \bar{V}_{j_\rho j_{\rho'}} . \quad (6)$$

Next we discuss how we treat the identical-nucleon systems. A generalized-seniority treatment would be most appropriate, particularly if we were interested in precise energies and occupation numbers. Our interest, however, is in the occupation numbers and in *corrections* to energies, and these can be obtained with essentially no loss of accuracy using the simpler BCS approximation. This is the method we have used in the calculation that we report in the following sections.

III. CALCULATIONS FOR NUCLEI JUST BELOW ^{208}Pb

A. Experimental input

As discussed in Sec. II, our method involves setting up an overcomplete system of coupled equations for the energy levels that depend only on the unknown p-n mme's of interest (as well as on additional "known" quantities). Each equation corresponds to a single experimental level. In principle, we could include all levels that to a good approximation have the appropriate generalized-seniority structure. Thus, in dealing with nuclei in the $Z = 50$–82, $N = 82$–126 shell, we could include levels just below ^{208}Pb as well as levels just above ^{132}Sn. All have the requisite structure and all depend on the same 30 mme's (corresponding to the five active proton orbits and the six active neutron orbits of this region). Unfortunately, there are insufficient experimental data available to carry out a simultaneous fit to all 30 effective mme's. Thus, it is essential to carry out the analysis in steps, focusing in each on those nuclei for which a limited number of mme's are expected to dominate.

We will in this work focus on those nuclei that are just below ^{208}Pb. In particular, we will assume a ^{208}Pb doubly magic core (with bare single-particle energies given by the ^{207}Pb and ^{207}Tl spectra) and only consider those nuclei in which the dominant proton holes are in the $3s_{1/2}$, $2d_{3/2}$, and $1h_{11/2}$ orbits and the dominant neutron holes in the $2f_{5/2}$, $3p_{1/2}$, $3p_{3/2}$, and $1i_{13/2}$ orbits. Nuclei for which this is the case (and which should also have the appropriate generalized-seniority structure) are those of the odd- and even-Hg isotopes and the odd-Tl isotopes. To a good approximation, the energies of these levels should depend on only 12 of the p-n mme's. As we will discuss shortly, in the end we were able to extract reliable estimates for 8 of the 12.

The even-Hg binding energies can be readily extracted from existing compilations [16]. The choice of energies in odd-mass nuclei, however, is more subtle and requires significantly more care. In odd-mass nuclei, some mixing of generalized seniorities can occur even for semimagic systems. This leads to a fragmentation of single-particle strength, as reflected by single-nucleon pickup spectroscopic factors. Ideally, we should use the centroid of pickup strength to represent the energies of the unmixed pure-generalized-seniority configurations. Unfortunately, sufficient data do not always exist. This is in part due to the difficulty of resolving states at higher excitation energies, in part to the inability to assign reliable J^π values (particularly regarding $l \pm 1/2$ ambiguities), and in part to the inherent unreliabilty of small spectroscopic factors. Of equal importance, even if complete and reliable data were available in some nuclei in an isotopic chain, there are often other nuclei that are simply inaccessible with transfer reactions. It is clearly inappropriate to use complete centroids in some nuclei in a chain and then to switch to the lowest levels of a given spin and parity in another.

All of these issues have led us, after many trials and sensitivity tests, to develop a set of rules and procedures for choosing a consistent set of data for the odd-mass nuclei included in our fits. First, only major components of the spectroscopic strengths were included in the extraction of centroids. Second, all orbits with extensive fragmentation (e.g., the $d_{5/2}$ proton orbit in Tl) were not included in the fits. The results that we will report are based on this set of rules. However, we have also carried out calculations using instead the lowest states of each spin and parity. The fact that the results obtained from the two separate fits were not very different convinces us that our prescription is relatively stable.

There are a few other points worth mentioning here. Even among the odd- and even-Hg isotopes and the odd-Tl isotopes, there are some nuclei that should not be included in the fit. In the lighter isotopes, the $\pi(h_{9/2})$ orbit begins to "intrude" into the low-energy spectra (also as a consequence of the monopole p-n interaction) [7], producing the onset of collective behavior. Once this occurs, the low-lying states no longer have the desired simple generalized-seniority structure, nor do they depend solely on the mme's of interest. As a consequence, we have not included data for $A < 195$ in our fits. At the other extreme, we also do not include the nucleus ^{205}Tl, since we do not expect a coherent generalized-seniority structure to evolve for a nucleus with so few valence neutrons and protons.

Figure 2 compactly summarizes the nuclei and effective single-particle levels that were used in the fits. The caption gives details. One of the end results of this study will be the recognition that a more thorough approach to the problem of p-n mme's necessitates more extensive data, even for the limited region of nuclei just below ^{208}Pb. We will return to this later.

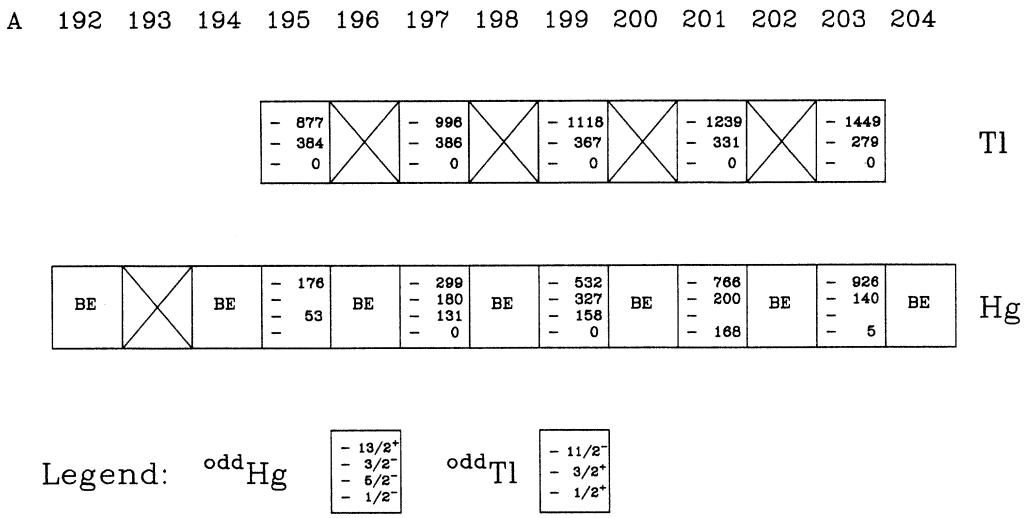

FIG. 2. A schematic summary of the data included in the fit, in the form of a slice of the nuclear chart (see text for a more detailed discussion). The notation BE in the boxes for the even-Hg isotopes denotes the binding energy relative to ^{208}Pb. For odd-A nuclei, the ground state binding energies are also included in the fits, as are the effective single-particle energies shown in the respective boxes (in keV). The format for the effective single-particle levels is given in the legend. Note that this format, which applies for all odd-mass nuclei included in the fits, does not imply an ordering in energies of these levels. Boxes criss-crossed by an $\times$ indicate nuclei for which no data were used.

B. Further details and results

In addition to the experimental data described above, the other crucial ingredients to our calculations are appropriate pairing strengths. These, in conjunction with the p-n mme's, dictate the distribution of particles in the states included in the fit. We have considered two prescriptions for the pairing strengths:

$$\text{I}: \quad G_p = \frac{18}{Z}, \quad G_n = \frac{18}{N},$$
$$\text{II}: \quad G_p = \frac{17}{A}, \quad G_n = \frac{23}{A}.$$

Prescription I is favored by calculations of quasiparticle energies in the Pb region, while II is perhaps the most commonly used. Solutions to the system of equations [(3)–(5)] showed a preference for the latter prescription: The rms deviations between fitted and experimental levels with prescription I were typically about 30% larger. We therefore adopt prescription II in the analysis to follow, although we feel that further study of this issue is worthwhile.

Even with the data limited to nuclei relatively near ^{208}Pb, the calculations still in principle involve all 30 mme's. However, since the nuclei we include have very few holes in the lower levels, their low-lying energy levels are not sensitive to the corresponding 18 mme's. We tried several prescriptions for these other mme's and found that, for any reasonable choice, the values extracted for the important mme's and their associated errors were more or less the same. In the results to follow, we set, for definiteness, all 18 mme's involving the $\pi(2d_{5/2})$, $\pi(1g_{7/2})$, $\nu(2f_{7/2})$, and $\nu(1h_{9/2})$ orbits to -0.2 MeV.

As noted earlier, of the 12 matrix elements corresponding to the upper single-particle orbits, only 8 could be determined accurately from the levels included in the fit. The other four, involving the p-n pairs $\pi(2d_{3/2})$-$\nu(1i_{13/2})$, $\pi(1h_{11/2})$-$\nu(1i_{13/2})$, $\pi(2d_{3/2})$-$\nu(3p_{3/2})$, and $\pi(1h_{11/2})$-$\nu(3p_{3/2})$, invariably emerged from the fits with very large uncertainties. We fixed these four matrix elements at the following values (all in MeV):

$$\bar{V}^{p\text{-}n}_{2d_{3/2}\text{-}1i_{13/2}} = -0.20\ ,$$
$$\bar{V}^{p\text{-}n}_{1h_{11/2}\text{-}1i_{13/2}} = -0.40\ ,$$
$$\bar{V}^{p\text{-}n}_{2d_{3/2}\text{-}3p_{3/2}} = -0.30\ ,$$
$$\bar{V}^{p\text{-}n}_{1h_{11/2}\text{-}3p_{3/2}} = -0.20\ ,$$

reflecting the general belief [1,13] that mme's corresponding to p-n pairs with similar quantum numbers (and particularly those with large and similar quantum numbers) should be stronger than those for which the quantum numbers differ substantially. However, we have checked that the final results were not very sensitive to the detailed choices.

Ultimately, the calculations that we carried out involved fits to 38 experimental data with 8 unknown mme's. Convergence of the iterative solution to (3)–(5) was usually quite rapid (typically < 5 iterations), and both the rms deviations of the fits and the resulting mme's were not very sensitive to further details of the calculations (e.g., we could remove some of the less certain levels from the fit or we could fix the unvaried mme's at alternative values without substantially changing the results).

Our final results are summarized in Table I. The overall rms deviation of the fit was 116 keV. We also include statistical errors for each of the fitted mme's. Note that

TABLE I. Effective p-n monopole matrix elements arising from a fit to 38 energy levels in the even-Hg isotopes and the odd-Hg and -Tl isotopes, as described in the text. In parentheses are given the statistical errors associated with each calculated matrix element. All matrix elements involving the $2d_{5/2}$ and $1g_{7/2}$ proton orbits and/or the $2f_{7/2}$ and $1h_{9/2}$ neutron orbits were set to -0.2 MeV and not included in the fit. Others that were not included in the fit are denoted by (n.f.) for the error. All results are given in MeV.

J_p/J_n	$3p_{1/2}$	$2f_{5/2}$	$3p_{3/2}$	$1i_{13/2}$
$3s_{1/2}$	-0.47 (0.02)	-0.37 (0.01)	-0.09 (0.04)	-0.30 (0.02)
$2d_{3/2}$	-0.62 (0.06)	-0.21 (0.04)	-0.30 (n.f.)	-0.20 (n.f.)
$1h_{11/2}$	-0.30 (0.12)	-0.39 (0.06)	-0.20 (n.f.)	-0.40 (n.f.)

in all cases they are substantially smaller than the matrix elements themselves. As such, we can conclude that all 8 mme's have been determined to a fair degree of accuracy. We should emphasize that the errors listed are from the fits alone and do not include contributions from uncertainties in the remaining input parameters (e.g., pairing strengths, the use of centroids vs lowest spe's, etc.).

G-matrix results for the p-n mme's appropriate to this region were reported some time ago in Ref. [7] (Table I). On the average our semiempirical mme's are somewhat weaker than those of Ref. [7]. There are also some rather glaring differences in specific mme's, most notably in the interaction between a $3s_{1/2}$ proton and a $3p_{3/2}$ neutron. Our value for this matrix element is -0.09 MeV, whereas the G-matrix calculation gives -0.79 MeV. It is interesting to note that when the matrix elements of Ref. [7] (supplemented by the common value of -0.2 MeV for those not listed) were inserted into the system of equations (3)–(5), the resulting rms deviation was 2.56 MeV. This reinforces our earlier comment that first-principles treatments to date have not been able to produce reliable p-n mme's, and underscores the importance of empirical extractions of monopole p-n matrix elements.

The less-comprehensive fits of Ref. [9] also produced values for several of the same matrix elements that we have determined, notably for those involving the $3s_{1/2}$ proton orbit. In general, the two sets of calculations give similar results for these matrix elements, even though our analysis included more data in the fits and also incorporated effects of the p-n monopole interaction in modifying the identical-nucleon contributions to the energies.

IV. CONCLUDING REMARKS

In this paper, we describe a method to extract effective proton-neutron monopole matrix elements from experimental data. The method is based on the observation that for nuclei in which at least one type of nucleon is near a closed shell, the low-lying states should have a simple generalized-seniority structure, whereby the neutrons and/or the protons have $J^\pi = 0^+$. In such nuclei, the only component of the proton-neutron interaction that contributes is the monopole. The energies of such states can be expressed in terms of quantities that can either be extracted from data or reliably calculated, and the unknown monopole matrix elements. These unknown quantities can then be obtained from a nonlinear least-squares fit to the experimental energies.

We have applied this method to nuclei just below ^{208}Pb, where enough experimental data exist to reliably pin down several mme's. The calculations yield fairly definitive predictions for 8 mme's, corresponding to the last few proton and neutron orbitals in the $Z = 50$–82 and $N = 82$–126 shells, respectively.

The extracted matrix elements, all of which have fairly small statistical uncertainties, in general seem reasonable. They are all attractive and on the average exhibit the property that those corresponding to neutron and proton orbits with similar quantum numbers are stronger than those for which the quantum numbers differ substantially.

The matrix elements that we obtain are on average somewhat smaller than those from first-principles G-matrix calculations. This we believe is essential if we wish to describe not only excitation spectra but also binding energies. And indeed effective shell-model-type fits in heavy nuclei [17] lead to magnitudes similar to those we obtain.

It is our hope that reliable effective p-n matrix elements, extracted from experimental data as in our analysis, can provide useful constraints for models (microscopic or otherwise) that attempt to understand the evolution of single-particle energies in the nuclear shell model. Since these single-particle energies are critical to a quantitative understanding of nuclear structure, both near and far from stability, such constraints should prove very useful, particularly as new realms of nuclear species become accessible in the future.

The proposed method can in principle be used to obtain all p-n mme's for heavy nuclei, where the valence neutrons and protons fill different major shells. In lighter nuclei, proper consideration of isospin conservation would lead to some mixing of generalized-seniority configurations.

While it may be possible to extract a few more mme's in heavy nuclei at this time, the feasibility of using our method to systematically determine *all* mme's hinges on the availability of significant new experimental data. Radioactive beam facilities, of the type currently being proposed, may provide the required experimental tool.

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