Semirealistic shell-model interaction for neutron hole states in ^{208}Pb†

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The Brueckner G matrix from the Reid soft-core potential is taken for the leading contribution to the effective two-neutron hole interaction in the ^{208}Pb region. To accomodate the corrections expected from core polarization and other higher order effects, including truncation of the model space, we add phenomenological two-body pairing and multipole forces whose strengths are determined by fitting the ^{206}Pb spectrum. A satisfactory fit is obtained with an interaction where the average total contribution of the added terms is less than 45% of the interaction. The same total effective interaction is then shown to yield a satisfactory spectrum for ^{204}Pb which may indicate the neglected effective many-body forces are not important. A comparison with the results of McGrory and Kuo is presented to examine the impact on the effective interaction of limiting the model space. We conclude the prospects are good for extending this approach to other nuclei below ^{208}Pb viewed as shell-model systems of valence holes in ^{208}Pb.

[NUCLEAR STRUCTURE Shell-model structure of Pb isotopes; theory of shell-model effective interaction with phenomenological corrections; multipole potentials added to Brueckner reaction matrix.]

I. INTRODUCTION

Traditional efforts to study the nuclear shell model have been, for the most part, divided into two main categories. In the first group the effective interaction is taken as a purely phenomenological force. Examples include a pairing plus quadrupole force,[1] a surface δ[2] or modified surface δ[3] interaction, other forms of density dependent interactions,[4] and simple Yukawa, Gaussian, and δ function forces with various spin and isospin exchange strengths. The central goal of these efforts is to produce spectra and transition properties in agreement with experiment at the sacrifice of full understanding of the microscopic origin of the effective interaction.

In the second category we include those efforts whose central goal is a microscopic derivation of the effective shell-model interaction from the basic nucleon-nucleon interaction. Here, agreement with experiment is but a hope which has not been achieved to a satisfactory extent. In the predominant theory the effective interaction is expressed as an expansion in powers of the Brueckner reaction matrix[5] G. A number of fundamental problems such as the convergence rate of the expansion[6] and the slow convergence of intermediate state sums[7] remain to be solved. It is significant, for our purposes, to note that these problems are associated with higher order terms in the expansion.

Attempts to bridge the gap between these two domains have been few. Freed and collaborators[8,9] employed the Tabakin[10] force with phenomenological corrections in the Pb region with some success. Nishibori[11] has also studied this approach in cases of only two valence nucleons. With the precision now available for calculating the Brueckner G matrix for valence model spaces in heavy nuclei and with the preeminence of the Pb region for shell-model behavior, we argue a renewed investigation of this semirealistic approach to these nuclei is needed. The central goal here is to obtain some insight into the required higher order corrections to the microscopically derived effective interaction and, simultaneously, achieve spectra and wave functions in reasonable agreement with available data. Another aim is to deduce a semirealistic interaction for a suitable model space to eventually extend shell-model investigations as far as the open-shell nuclei in the vicinity of $A = 200$.

Within the context of these goals, previous shell-model studies with realistic forces bear some import. Kuo and Herling[12] evaluated the effective interaction for the Pb region through second order in G and studied systems with two valence particle or two valence hole degrees of freedom about the ^{208}Pb core. Some spectra they obtained were reasonable even though the adequacy of the theoretical methods is doubtful.[6,7] Recently, McGrory and Kuo[13] (hereafter referred to as MK) employed the Kuo-Herling realistic matrix elements to study nine nuclei in the vicinity of ^{208}Pb. In a number of these nuclei they found it desirable to invoke phenomenological adjustments to obtain improved agreement with experiment.

We shall concentrate on ^{204}Pb and ^{206}Pb in this

TABLE I. Neutron hole energies near ^{208}Pb.

Neutron orbital	Single hole energy (MeV)
$2p_{1/2}$	0.0
$1f_{5/2}$	0.570
$2p_{3/2}$	0.898
$0i_{13/2}$	1.633
$1f_{7/2}$	2.340
$0h_{9/2}$	3.409

initial effort for two reasons. First, our approach must be proven adequate for these relatively simple cases if we are to have confidence in predictions for more complex nuclei. Second, the comparison of our results in a smaller model space with those of MK permit additional insight into and confirmation of our methods.

II. MODEL SPACE AND EFFECTIVE HAMILTONIAN

With only two or three neutron holes it is not difficult to perform shell-model calculations with all configurations within the entire last major neutron shell of ^{208}Pb. However, with only four neutron holes some matrices already exceed 500 $\times$ 500. This implies that calculations for $A = 200$ which include an entire shell for both neutron and proton holes are not presently feasible. Thus we investigate the possibility that the major features of the low-lying spectra may be explained in a smaller model space. Even if this possibility is realized for our limited space, matrices larger than 500×500 will occur for the $A = 200$ nuclei. The smaller model space renders the $A = 200$ problem tractable although considerable computing resources will still be required.

Table I presents the experimental single hole energies for neutron holes in the last major shell at $N = 126$. MK employed all six orbitals and essentially these energies in their calculations. We employ only the $2p_{1/2}$, $1f_{5/2}$, and $2p_{3/2}$ orbits with the experimental energies presented in Table I.

The effective shell-model interaction is assumed to be purely two body in character and is comprised of two additive parts. The first is obtained by microscopic theory from the basic nucleon-nucleon interaction while the second is phenomenological and obtained in various fitting procedures as described below.

The theoretical component is the Brueckner reaction matrix[5] G, obtained from the Reid soft-core nucleon-nucleon potential.[14] This is taken as the leading term in the Bloch-Horowitz-Brandow[15] expansion for the realistic effective shell-model interaction. It was originally obtained for Hartree-Fock-Bogoliubov studies of rare-earth nuclei[16] but has also been shown to be useful in other applications to nuclei from Sn to Pb.[16-18] Since it has been discussed in some detail in Ref. 16 we only mention its chief features here for completeness. The G matrix is obtained in an oscillator single-particle basis (oscillator constant $\hbar\Omega = 7.5$ MeV), so the Pauli operator is treated exactly. For the purpose of the rare-earth studies a very large model space was chosen. The Pauli operator is of the shell-model type with an inert core of 40 neutron and 40 proton orbitals. The valence space extends through the next 96 orbitals of each isospin so it even includes the $1g_{9/2}$ orbital above the shell closure at 126 particles. This model space is, of course, significantly larger than the choice for the present application. One could correct for this discrepancy in principle by adding higher order terms to the effective interaction expansion. However, this was not felt to be warranted since the other higher order terms will be parametrized.

For the Hartree-Fock problem the starting energy ω should be chosen self-consistently. For the valence space Hartree-Fock application it was shown that a single-particle energy of -10 MeV was a good approximation to the average self-consistent result. This was the value used to solve for $G(\omega)$. In a shell-model application such as the present case, this value of ω signifies there is a shift of 10 MeV between the valence space oscillator states and the unoccupied states.[19] There is some theoretical and some empirical motivation for a shift of this nature.[19]

Perhaps one of the more salient limitations of the G matrix we employ is due to the absence of partial waves of the Reid soft-core potential for total relative angular momentum $\mathcal{J} > 2$.

The second element of the effective Hamiltonian is a parametrized two-body interaction to be added to the G matrix in order to accommodate the neglected higher order effects including those arising from truncation of the model space. Our hope is that the parametrized corrections will be small in comparison with the G matrix contribution to the effective Hamiltonian. Indeed, these empirical corrections are found to exceed 100 keV for less than 25% of the matrix elements.

The simple parametrization adopted here has been successfully employed in the Pb region by Freed and various co-workers[8,9] and by Nishibori.[11] It consists of a pairing force plus multipole forces with adjustable strengths. The former groups employed the Tabakin interaction and adjusted the strengths of these added terms to best produce the low-lying spectra of nuclei having two valence particles and/or holes around the ^{208}Pb core. They were then able to add one more parti-

cle or hole and obtain exceptionally good spectra with no further adjustment of the strengths. Nishibori's results using the Hamada-Johnston[20] potential are slightly more difficult to evaluate since he did not consider cases more complex than the two-body case and did not actually select specific values for his strength parameters.

The multipole forces used here are P_n $(n=2,4)$, where

$$P_n = -X_n r_1^n r_2^n \mathcal{P}_n(\cos\theta_{12}),$$

where $\mathcal{P}_n$ are the Legendre polynomials, $\vec{r}_1$ and $\vec{r}_2$ are coordinates of the interacting nucleons, and θ_{12} is the angle between $\vec{r}_1$ and $\vec{r}_2$. Thus our P_2 force is essentially the two-body part of the Elliott or SU3 quadrupole-quadrupole operator. The two-body matrix elements of P_n are

$$\langle j_a j_b J | P_n | j_c j_d J\rangle = -X_n[(1+\delta_{ab})(1+\delta_{cd})]^{-1/2}[(2j_a+1)(2j_b+1)]^{1/2}(-1)^{j_a+j_d}$$
$$\times[(-1)^J\langle r^n\rangle_{ac}\langle r^n\rangle_{bd} W(j_a j_b j_c j_d;Jn) C^{j_a\, n\, j_c}_{1/2\, 0\, 1/2} C^{j_b\, n\, j_d}_{1/2\, 0\, 1/2} + \langle r^n\rangle_{ad}\langle r^n\rangle_{bc} W(j_a j_b j_d j_c;Jn) C^{j_a\, n\, j_d}_{1/2\, 0\, 1/2} C^{j_b\, n\, j_c}_{1/2\, 0\, 1/2}].$$

This expression is for like particles. For unlike particles the δ's and the second term in the last bracket vanish. The expectation values of r^n are computed using harmonic oscillator functions. Our pairing force is the one used by Kisslinger and Sorensen.[1] Its matrix elements are

$$\langle j_a j_b J | V_{\text{pairing}} | j_c j_d J\rangle = -\tfrac{1}{2} X_0 \delta_{J0}\delta_{ab}\delta_{cd}(-1)^{j_a+j_c}[(2j_a+1)(2j_c+1)]^{1/2}.$$

It has been previously shown by Brown and Kuo[21] that core-polarization corrections for Ni matrix elements bear a marked similarity to a sum of pairing and P_2 matrix elements. They also state that an important P_4 contribution is present. With properly choosen parameters we show below that this phenomenological force can also be a good approximation to the MK core-polarization corrections in the lead region.

III. RESULTS AND DISCUSSION

A. Effective Hamiltonian

Figure 1(a) shows the similarity between the $T=1$ bare interaction matrix elements of MK and of this effort. Only those required for our small model space are displayed. Note that there is substantial agreement between the two sets except that our G matrix is systematically stronger.

In addition to some calculations using just their bare interaction, MK also reported some spectra for an effective interaction renormalized by second order corrections. They included microscopically calculated terms for the 3h-1p and 4h-2p processes. For the ^{204}Pb and ^{206}Pb spectra, they found it expedient to multiply the 3h-1p term by 0.75 and to drop the 4h-2p term altogether in their final calculation, which could be considered further justification for the philosophy of the present approach.

Since we hope to simulate higher order effects with simple pairing plus multipole forces, it is natural to ask how well such a treatment can reproduce the results of a microscopic calculation. To answer this question we carried out a least squares fit of pairing plus P_2 and P_4 to the adjusted microscopic core-polarization matrix elements of McGrory and Kuo. The results are shown in Fig. 1(b) plotted on the same scale as Fig. 1(a). In most cases the differences are small compared to the size of the bare interaction. The rms deviation between the MK results and the simple simulation is only 29 keV.

If we allow only pairing and P_2 terms in the fit the quality of the fit is about the same. Although the strength parameters change considerably the rms deviation increases only to 39 keV. This leads us to conclude that the P_4 term is not as essential for the MK core-polarization term. On the other hand, we do find it plays a significant role in achieving acceptable shell-model spectra for ^{204}Pb and ^{206}Pb in the limited model space. Thus, P_4 appears to be more closely connected with those higher order effects arising from the substantial model space truncation. This will be further clarified in analyzing the spectra presented below.

In Fig. 1(c) we compare the matrix elements of pairing plus P_2 and P_4 obtained in the fit (limited model space) to the ^{206}Pb spectrum with the adjusted core-polarization results of MK. Overall, these contributions are still small by comparison with the bare interaction. The differences in Fig. 1(c) could be interpreted as a measure of the effects of model space truncation since each contribution to the effective interaction in their respective model spaces produces reasonable spectra.

As a quantitative indication of the corrections in comparison to the bare matrix elements we define

$$\Delta = \frac{\sum|\text{correction}|}{\sum|\text{total}|},$$

where the summation is over the matrix elements of the small model space. For the MK matrix

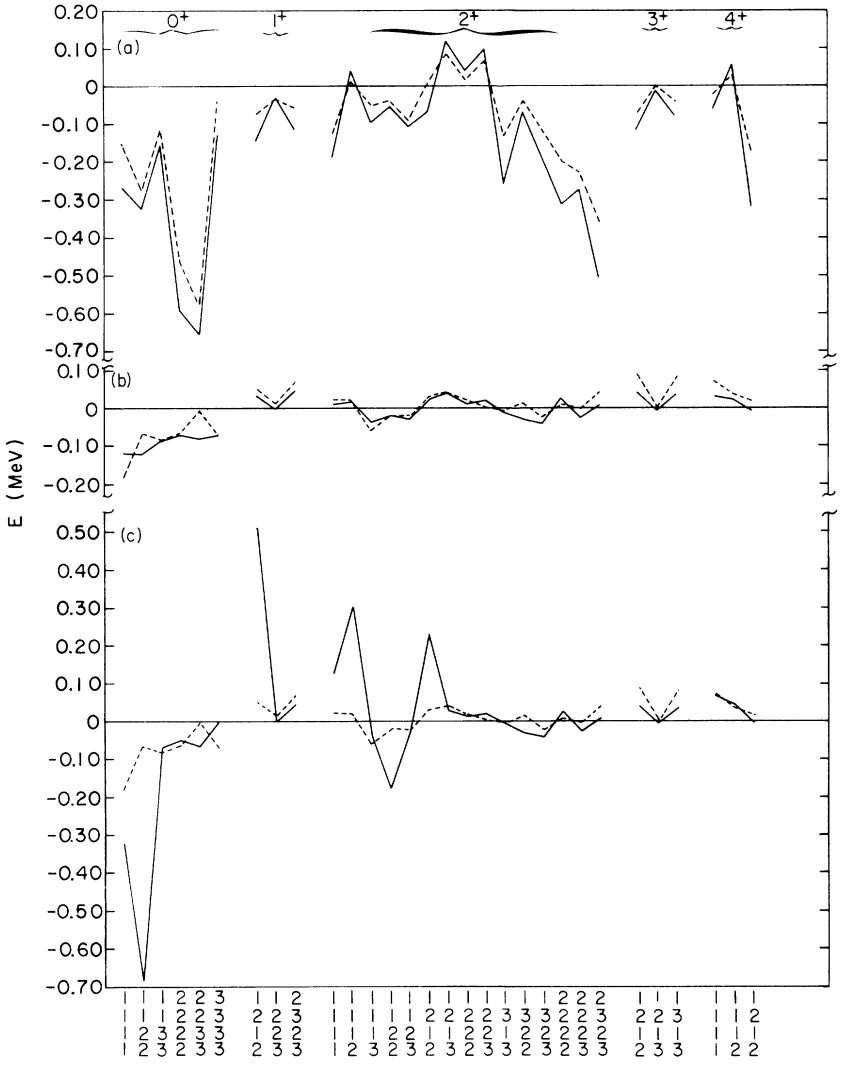

FIG. 1. ^{206}Pb matrix elements. All two-body matrix elements of the small model space are shown. J is given at the top of the figure while the labels of each matrix element are given at the bottom: $1 = 1f_{5/2}$, $2 = 2p_{3/2}$, $3 = 2p_{1/2}$; (a) bare matrix elements; solid line connects our G matrix elements, dashed line connects bare matrix elements of MK; (b) pairing plus P_2 and P_4 (solid line) fit to MK-adjusted core polarization (dashed line); (c) pairing plus P_2 and P_4 matrix elements obtained in fit to ^{206}Pb spectrum (solid line). Dashed line is again MK-adjusted corrections.

elements and for our case where X_0, X_2, and X_4 were determined by fitting MK's corrections, Δ is about 0.19. When the parameters were fixed by fitting to the experimental ^{206}Pb spectrum, Δ increased to 0.42. Much of this change is concentrated in a few matrix elements.

Table II summarizes the multipole strength parameters obtained in the various fits. Note that there are significant variations in the individual strengths and this is also reflected in the large uncertainties quoted adjacent to the strengths obtained in the χ^2 fits to MK matrix elements. A study of the error matrix reveals large correlated uncertainties between the parameters. Thus, a significant tradeoff between pairing, P_2 and P_4 terms may be obtained. The net conclusion is that higher order corrections (excluding those related to model space truncation) to the effective interaction required by the data are small as compared with the bare interaction and are somewhat uncertain as to their multipole content.

B. Spectra of ^{206}Pb and ^{204}Pb

We have not performed any calculations in the larger model space used by MK but we can isolate the effects of our small model space by truncating

TABLE II. Multipole strength parameters.

		X_0	X_2	X_4
Fit to MK core polarization	Fit(a)	0.0114 ±0.0070	0.001 32 ±0.000 24	0.629×10^{-5} $\pm0.148\times10^{-5}$
	Fit(b)	0.0288 ±0.0064	0.926×10^{-3} $\pm0.250\times10^{-3}$	
Fit to experiment		0.003 00	0.001 30	0.550×10^{-4}

their matrices. In Fig. 2 the columns (e) are the MK results while columns (b) are results of the same effective Hamiltonian truncated to our small model space. Columns (b) have been positioned to minimize the rms deviation from experiment. Notice that although the agreement with experiment does suffer somewhat, the smaller model space still predicts the approximate ordering and density of low-lying levels in ^{206}Pb and ^{204}Pb. The larger model space is unable to correct features such as insufficient spacing between 3_1^+ and 2_2^+ or the disagreement in the 1_1^+ and 4_1^+ levels of ^{206}Pb.

Comparisons between our work and MK are difficult to evaluate because any given effect could be caused by the difference in effective Hamiltonians or model spaces or both. A calculation was made to find out how well the pairing plus multipole forces can compensate for the truncation. We added pairing and P_n forces to the MK bare plus (adjusted) microscopic core polarization matrix elements in our small model space. The strengths were adjusted to fit the ^{206}Pb spectrum McGrory and Kuo obtained in their large model space calculation. When only pairing and P_2 forces are included in the small space calculation the rms deviation between large and small model space results is 90 keV. If the series of multipole forces is extended to include the P_4, then the agreement improves to an rms deviation of only 30 keV. These contrast with an rms deviation between ^{206}Pb spectra using the large and small model spaces (without pairing and multipole forces) of

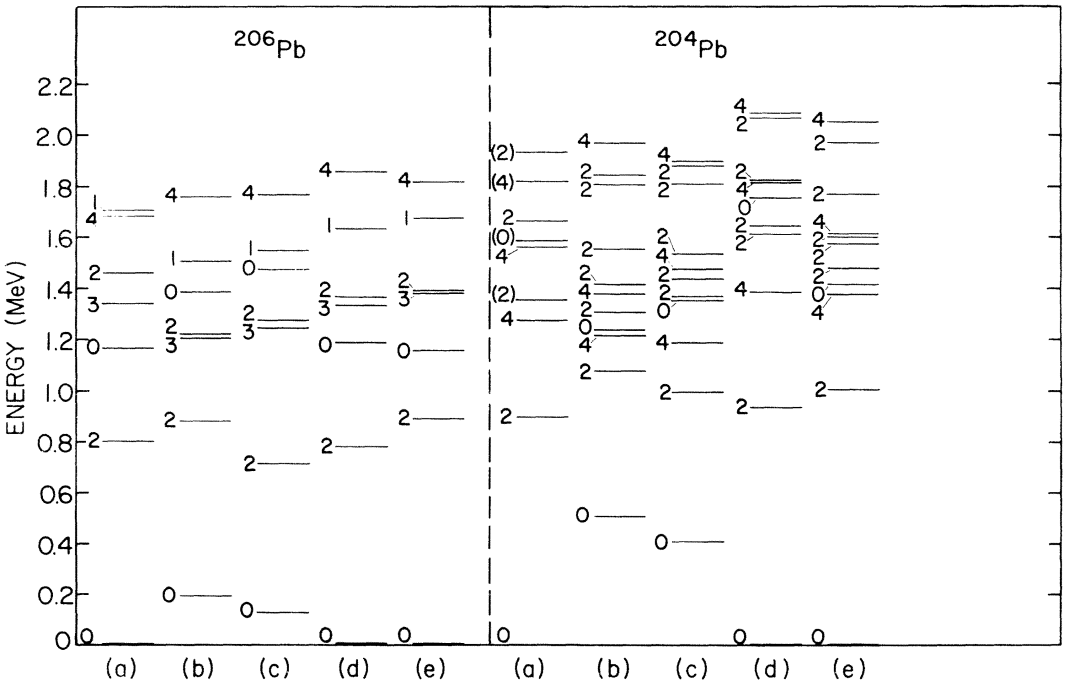

FIG. 2. ^{206}Pb and ^{204}Pb spectra obtained from (a) experiment (Ref. 21); (b) MK matrices truncated to small model space; (c) effective interaction with pairing plus P_2 and P_4 fit to MK-adjusted corrections; (d) effective interaction with pairing plus P_2 and P_4 determined by fitting ^{206}Pb spectrum; (e) MK calculation using large model space and adjusted core polarization.

TABLE III. Binding energies and deviations from experiment. Spectrum labels refer to Fig. 2. Experimental ground state energies are determined from binding energy data. $E(^{206}\mathrm{Pb}) = \mathrm{B.E.}(^{208}\mathrm{Pb}) - \mathrm{B.E.}(^{206}\mathrm{Pb}) + 2[\mathrm{B.E.}(^{207}\mathrm{Pb}) - \mathrm{B.E.}(^{208}\mathrm{Pb})]$, and similarly for ^{204}Pb.

Spectrum	Ground state energy (keV)	rms deviation from experiment [a] (keV)
	^{206}Pb	
a(Expt)	-627 ± 93	
b	−406	174
c	−592	167
d	−805	80
e	−770	67
	^{204}Pb	
a(Expt)	-547 ± 187	
b	−183	234
c	−1050	173
d	−1672	167
e	−1220	163

[a] Theoretical spectra shifted to minimize.

160 keV. Thus it appears that added terms to allow for the model space truncation are justified and that the P_4 force plays a significant role in this respect.

If one uses the small model space and our bare matrix elements plus the (pairing $+P_2+P_4$) force determined by fitting to the microscopic core polarization, one would expect to obtain spectra in good agreement with the spectra of columns (b) in Fig. 2. Columns (c) of Fig. 2 show the results of such a calculation. For ^{206}Pb columns (b) and (c) are indeed very similar and they have about the same agreement with experiment. For ^{204}Pb columns (b) and (c) are again similar, although most level spacings are modified.

A more significant test of our method consists in fitting the strengths directly with the experimental ^{206}Pb spectrum and applying the result to ^{204}Pb with no further adjustment. The results are shown in columns (d) of Fig. 2. They are found to be rather comparable to experiment and to the final results of MK given in columns (e). It is interesting to note that our spectra agree with experiment almost as well as the MK spectra. We regard this as a strong validation of our conjecture that one could use a small model space with simulated higher order effects to obtain good predictions for the low-lying levels.

Table III contains additional information useful in the evaluation of the various spectra. In terms of rms deviation from experiment there is very little difference between spectra (d) and spectra (e). For ^{206}Pb all calculations yield ground state energies for the two neutron holes in reasonable agreement with experiment. For ^{204}Pb none of the predicted ground state energies is satisfactory. In both nuclei our effective interaction with the strengths determined by fitting to ^{206}Pb yields the most overbound prediction.

Additional support for our approach can be derived from the wave functions. Table IV summarizes the relevant information for the low-lying levels of ^{206}Pb and ^{204}Pb. For ^{206}Pb we obtain from 92% to essentially 100% of the wave function by using 17–50% of the configurations of the large model space. If one compares the ratio of wave-function overlap to the fraction of the large configuration space included in our calculations as an indication of the level of success, then the overlap of 0.95 obtained for the 4_1^+ level by employing only 17% of configurations of the large model space appears (as seems reasonable) as a much more impressive accomplishment than the overlap of 0.92 using 50% of the configurations of the MK model space for 0^+. From this viewpoint the use of only 3–8% of the large model space configurations to obtain overlaps of 0.53–0.91 for the low-lying levels of ^{204}Pb is more noteworthy. For both nuclei it appears that as J increases the fraction of the large space configurations contained in the small space decreases, but that the configurations present in the small space must become increasingly important as indicated by the overlaps.

IV. CONCLUSIONS

We have employed an approach to the nuclear shell model intermediate to purely phenomenological and purely microscopic calculations. This semirealistic approach has as its principal ingredient a G matrix determined from the Reid soft-core nucleon-nucleon interaction. Thus the leading term of the effective interaction is properly treated and we phenomenologically approximate only the higher order corrections which are expected to be small but significant and difficult to evaluate with precision. The pairing and multipole forces are very simple to use and have been shown capable of reproducing the limited available microscopic corrections to a satisfactory degree.

These calculations indicate that it is reasonable to expect good predictions of some of the principal features of low-lying spectra of lead region nuclei while using a model space of practical size. The success of the test cases prompts the extension to nuclei near $A = 200$.

We selected ^{206}Pb and ^{204}Pb as test cases because of their relative simplicity and because microscopic calculations in a large model space were available.[13] It is pleasing that our results are in good agreement with both experiment and the MK

TABLE IV. Comparison of wave functions.

Level	% of MK wave function contained in small space	Overlap of MK wave functions with those of this work	Size of matrix MK	Size of matrix Small space
		^{206}Pb		
0_1^+	85.7	0.919	6	3
0_2^+	87.6	0.917	6	3
1_1^+	~100.0	1.000	4	2
2_1^+	93.4	0.953	12	5
2_2^+	99.8	0.984	12	5
3_1^+	99.9	0.999	8	2
4_1^+	89.9	0.947	12	2
		^{204}Pb		
0_1^+	65.5	0.696	113	9
0_2^+	76.4	0.531	113	9
0_3^+	66.6	0.692	113	9
2_1^+	73.5	0.785	418	21
2_2^+	82.2	0.713	418	21
2_3^+	84.4	0.781	418	21
2_4^+	90.0	0.503 [a]	418	21
2_5^+	87.3	0.458 [b]	418	21
2_6^+	80.5	0.704	418	21
4_1^+	85.6	0.896	560	15
4_2^+	89.9	0.907	560	15
4_3^+	76.0	0.812	560	15

[a] 0.651 if 2_5^+ of MK is used.
[b] 0.697 if 2_4^+ of MK is used.

results. Detailed agreement with the latter was neither required nor expected but served to highlight features of our results.

Preliminary calculations for ^{202}Pb seem to indicate that the strength parameters determined by fitting ^{206}Pb may in fact require some adjustment as one moves further into the open shell.

We would like to acknowledge an enlightening private communication from M. Harvey on the various meanings which are frequently intended by the term "quadrupole-quadrupole force." Also, we wish to express appreciation to J. B. McGrory for extensive communication of the details of calculations reported in Ref. 13.

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