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WEAK-COUPLING CALCULATIONS IN THE ^{208}Pb CORE REGION

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The structure of Tl and Hg isotopes near the ^{208}Pb core is discussed in terms of a weak-coupling model where low-lying proton-hole states are coupled to low-lying neutron-hole states. The even Pb isotopes are first discussed in terms of a generalized seniority-2 approximation which is shown to be very accurate. The weak-coupling results are not satisfactory, and it is suggested that the defeat may be in the n-p interaction.

1. INTRODUCTION

With the development of heavy-ion beams and higher energy light-ion beams, the field of nuclear structure continues to be an exciting and expanding field. These new probes provide new information on nuclear states with large angular momenta and on states in nuclei far from stability. Such information has provided new challenges to nuclear structure theory, and it has offered new opportunities to study relationships between microscopic and collective nuclear models. In recent years, there has been much discussion[1] of the Interacting Boson Model (IBM) as a potential bridge between the microscopic and collective models. The IBM has been impressively successful as a phenomenological model which accounts for a wide variety of systematic data on nuclear properties. The microscopic foundation of the model is still under intense investigation, and there are many open questions. It would be extremely desirable to be able to perform some credible shell-model calculations of some nuclei which have been treated successfully by the IBM where the structure of the calculation is amenable to comparison to some of the IBM properties.

As an example of the sort of questions that might arise, a brief diversion to discuss the structure of the ^{208}Rn is in order. ^{208}Rn can be described as four proton-particles and four neutron-holes near an assumed ^{208}Pb core. There exist some data[2] on the low-lying states of ^{208}Rn, and the spectra have been described in terms of the IBM with apparent good success. In the IBM model of ^{208}Rn, there are two proton-particle bosons and two neutron-hole bosons. Thus, the states of ^{212}Rn which are included in the model space are the states generated by coupling two S and/or D bosons together, i.e. (J=0,sen-0), J=2,sen-2), and J=0,2,4, sen-4) states. Similar neutron-hole states in ^{204}Pb are included in the IBM model. The results of an IBM model calculation of ^{208}Rn are shown in Fig. 1, as is the experimentally measured spectrum. The calculated spectrum can be well correlated with the observed spectrum.

One can take a somewhat different view. One can say that as a first-order approximation, the neutron-proton interaction can be ignored, and that the spectrum of ^{212}Rn can be constructed simply by adding the observed low-lying spectra of ^{212}Rn and ^{204}Pb together. In the last column of Fig. 1, only those states are shown where the ground state of ^{204}Pb is coupled to the low-lying states of ^{212}Rn, or the ground state of ^{212}Rn is coupled to the spectrum of states in ^{204}Pb. There are, of course, many more excited states above ~ 1.8 MeV which would result from coupling two excited states together.

An entirely analogous "game" can be played for Po isotopes. Thus ^{208}Po = ^{210}Po × ^{206}Pb, and ^{206}Po = ^{210}Po × ^{204}Pb. Such "experimental" spectra are shown in the first two columns of Fig. 1. In all these spectra, dashed lines involve excited states in ^{210}Po or ^{212}Rn, while solid lines involve excited states in ^{206,204}Pb. Certainly for ^{208,206}Po, this very simple picture gives a good first approximation of the observed spectra. A modest n-p interaction could be expected to depress the first $J=2^+$ state to a position in agreement with experiment. Note the disappearance of a low $J=0^+$ between ^{208}Po and ^{206}Po which arises in the weak coupling model because the first $J=0^+$ state in ^{206}Pb is at a much lower energy than in ^{204}Pb. This in turn reflects the fact that the ground state of ^{206}Pb is predominantly $(p_{1/2}^{-2}, J=0)$ and the Pauli principle blocks the $(p_{1/2}^{-4}, J=0)$ configuration in ^{204}Pb.

Thus, two similar models account for the data. But there are very significant differences in the models. Consider first the Po isotopes. In ^{210}Po, in the IBM description, there are only two states -- the $J=0^+$ ground state or S boson, and the $J=2^+$ or D boson. In the observed spectrum of ^{210}Po, the lowest states have $J = 0^+-2^+-4^+-6^+-8^+$, and shell-model calculations indicate these are very pure $(g_{9/2}^{2})_J$ states. These $g_{9/2}^{2}$ states are the dashed lines in the spectra of ^{208}Po and ^{206}Po in Fig. 1, and there appear to be good analogs

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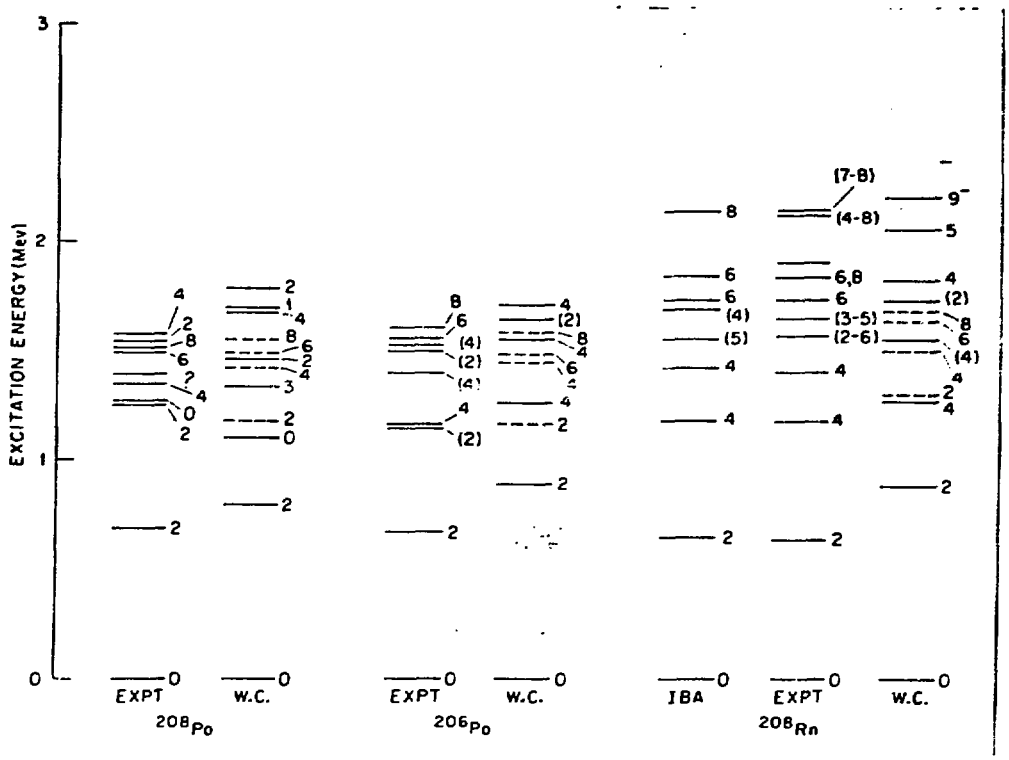

Figure 1 : "Experimental" weak-coupling spectra of ^{208}Po, ^{206}Po, and ^{208}Rn. Experimental spectra from Refs. 2 and 13. In the spectra labeled W.C. (weak coupling), dashed lines are excitation energies in proton systems and solid lines are excitation energies in neutron systems.

for these states in ^{208}Po. The weak coupling picture suggests these states are present in ^{206}Pb. In IBM parlance, these proton states are g-, i-, and k-bosons. The spectrum of low-lying states in ^{212}Rn is virtually identical to the spectrum of states in ^{210}Po. Again, shell-model calculations suggest these states are $(g_{9/2}{}^4)_J$ states, with seniority ν=0 for the J=0 states and ν=2 for the other states with J = 2, 4, 6, and 8. As discussed in Section 2 below, a similar situation exists in ^{204}Pb where all the low-lying states up to about 2.0 MeV excitation are ν=0 or ν=2 states. From this, it follows that only two $J=0^+$, two $J=2^+$, and one $J=4^+$ state in ^{208}Rn in the weak-coupling spectrum of ^{212}Rn in Fig. 1 can have any overlap with IBM states. The weak coupling picture is almost orthogonal to the IBM picture for ^{208}Rn. It raises serious questions here as to what extent is the IBM application to ^{208}Rn parameter fitting. Is this a case of applying the model to a system too close to a closed shell? An analogous situation occurs for the Pt isotopes. There is little experimental data in ^{204}Pt, the two-boson proton system. Shell-model calculations indicate all the low-lying states are ν = 0 or ν = 2, i.e., there are no low-lying, seniority-4, two-boson states in ^{204}Pt. A strong n-p interaction could "pull down" the seniority-4 states as more and more neutron holes are formed, thus accounting for the usefulness of the IBM away from closed shells. It would be interesting to see this transition occur in a more exact shell-model calculation.

In this brief report, I will discuss some calculations which are motivated by such questions. The calculations to date are both incomplete and not very successful, but they serve to illustrate some of the problems in such studies. The calculations focus on nuclei lighter than, but near, the ^{208}Pb closed-shell core. Some of the nuclei treated are isotopes of Tl, Hg, and Pt. In Section 2, the method of calculation is described and the parameters of the calculation discussed. In Section 3, truncation schemes for the neutron-hole states in the Pb isotopes are discussed. States in the Pb isotopes are building blocks in these calculations. In Section 4, the results of calculations of

^{205,203}Tl and ^{205,204,202}Hg are discussed. The results are summarized in Section 5.

2. METHOD OF CALCULATION

In the calculations discussed here, an inert ^{208}Pb core is assumed. Proton holes are allowed in the $s_{1/2}$, $d_{5/2}$, $d_{3/2}$, $s_{1/2}$, and $h_{11/2}$ orbits. Neutron holes are allowed in the $p_{1/2}$, $p_{3/2}$, $f_{3/2}$, $f_{7/2}$, $h_{9/2}$, and $i_{13/2}$ orbits. The dimensions in such a model space for more than three or four particles are impractically large, so some truncation scheme is required. We follow an approach discussed at length by Arima and Hamamoto[3] and used[4] with some success by Sau and Heyde in the mass ≈ 130 region, and by Strottman[5] for ^{212}Po among others. We work in an n-p formalism. Then, in an obvious notation

$$H = H_{pp} + H_{nn} + H_{np}.$$

First, H_{np} is ignored. In this lowest approximation, eigenstates of H are direct products of eigenstates of H_{nn} and H_{pp}. Thus, we first diagonalize H_{pp} and H_{nn} in the separate proton-hole and neutron-hole spaces, i.e.

$$H_{pp}|\psi_{pp}^{j}\rangle_{J_p} = E_p^j|\psi_{pp}^{j}\rangle_{J_p}$$

$$H_{nn}|\psi_{nn}^{j}\rangle_{J_n} = E_n^j|\psi_{nn}^{j}\rangle_{J_n}$$

A basis space is formed from the resulting neutron and proton eigenstates

$$|\psi_{p,n}^{i,j}\rangle_J = [|\psi_{pp}^{i}\rangle_{J_p} \times |\psi_{nn}^{j}\rangle_{J_n}]_J$$

Here the × indicates angular momentum coupling. Next, $H_{p,n}$ is diagonalized in the space of $|\psi_{p,n}^{i,j}\rangle_J$. If all eigenstates of H_{pp} and H_{nn} are included, this n,p space is complete, and no economy is achieved. One hopes that it is necessary to include only a relatively few low-lying proton and neutron states, thus achieving a practical number of basis states. In the calculations discussed here, we have started with the lowest neutron and proton eigenstates and then increased the number of basis states until there appears to be some degree of convergence. There is some reason to expect that only a relatively few low-lying states are needed. If H_{np} is weak relative to H_{pp} and H_{nn}, this should be so. Since the active neutrons and proton-hole states are in different single-particle orbits, the loss of single-particle wavefunction radial overlaps should lead to a diminution of the two-body matrix elements. Even in the sd shell, where neutrons and protons are in the same orbits, and where the n-p interaction is strong, the truncation scheme used here is reasonably successful.[6]

The parameters of the calculation are the single-hole energies and the two-body neutron-hole, proton-hole interaction matrix elements. The proton-hole and neutron-hole energies are taken from the observed spectra of ^{207}Tl and ^{207}Pb. As a starting point, the two-body realistic effective interaction matrix elements constructed[7] for the model space used here by Kuo and Herling were used. The two-neutron hole interaction has been empirically modified[8] by Blomqvist to improve agreement with experiment in ^{206}Pb and his modified interaction is used here. Further modifications of the interaction are discussed below.

3. TRUNCATION SCHEMES FOR THE Pb ISOTOPES

The first step in this weak coupling approach is to generate eigenstates in the neutron-hole and proton-hole spaces. We will deal here with isotopes of Tl and Hg, the systems with one- and two-proton holes, respectively. In these cases we diagonalize H_{pp} in the complete space. The neutron-hole systems in which we are interested are ^{206,204,202,200}Pb. Even for these identical-particle (or maximum isospin) systems, the model space is too large to handle exactly, so some form of truncation is needed. One can use a "cluster" approach to this problem, as was done[9] by Ko, *et al.*, and more recently has been pursued[10] by Pomar and Liotta, Boisson and Silvestre-Brac, among others. As an example of this approach, consider a calculation of ^{204,206}Pb. One can find the exact eigenstates of ^{206}Pb by diagonalization in the complete two-hole space. From this calculation, define a two-particle state creative operator $Z_{J_i}^{E_i}$ which, when operating on the ^{208}Pb "vacuum", creates an eigenstate of ^{206}Pb with angular momentum J_i and energy E_i, i.e.

$$|E_i,J_i\rangle = Z_{J_i}^{E_i}|^{208}\mathrm{Pb}\rangle$$

where

$$Z_{J_i}^{E_i} = \sum_{j_1 j_2} \alpha_{j_1 j_2}^{E_i,J_i}(a_{j_1} \times a_{j_2})^{J_i}$$

and a_{j_1} is the usual destruction operator for the orbit j_1. One can then create creation operators for ^{204}Pb states by coupling together two ^{206}Pb creation operators, i.e.

$$Z_{J_1,J_2}^{E_1,E_2} = \left[Z_{J_1}^{E_1} \times Z_{J_2}^{E_2}\right]^J$$

In this case, the operators involve equivalent particles, so the Pauli principle becomes a

factor. If one includes all possible two-particle states, an overcomplete and non-orthogonal basis is generated. One can, however, construct an orthonormal basis in terms of these operators. The approach is useful if one need only include a few two-particle states. We discuss a few results below in this approach. This cluster approach obviously has some analogy with the IBM approach. One might consider only the first 0^+ and 2^+ states in ^{206}Pb and identify these states as S and D "two-Fermion" operators. These operators might then be identified with the S and D bosons of the IBM.

A second approach is to restrict the shell-model calculation basis space to those configurations where the sum of the seniorities of all pure configurations is less than 2. With this restriction, calculations of the even Pb isotopes down to ^{198}Pb are manageably small. It has already been[11] shown that such an approximation in ^{204}Pb is in very good agreement with the exact diagonalization result. In Fig. 2 we compare these truncation schemes for $J=0^+$, 2^+, and 4^+ states in ^{204}Pb, and $J=0^+$, 2^+, 4^+, and 6^+ states in ^{202}Pb. For ^{204}Pb we show the observed spectrum, the results of an exact diagonalization in the four-hole space, the results where the seniority-2 truncation is used, and two cluster calculations. In the cluster results[9] of Ko, *et al.*, the lowest four states in ^{206}Pb are included in the basis. In the calculation[10] of Pomar and Liotta, the lowest 50 two-cluster states in ^{204}Pb in zero order (before diagonalization) are included. One can see that: 1) the exact calculation is in excellent agreement with experiment, 2) except for the third $J=4^+$ state, the seniority-2 calculation is in very good agreement with experiment, 3) the Ko, *et al.* calculation is too truncated, 4) the Pomar-Liotta results are in reasonable agreement with the exact diagonalization, although there is an indication there are extra states at low energy in the Pomar-Liotta calculation. For ^{202}Pb, only two calculations are shown. One is the $v=2$ calculation. The second is one by Pomar and Liotta,[10] where the lowest 20 states in zero order found from coupling ^{204}Pb states to ^{206}Pb states are included. The seniority-2 calculations are in good agreement with our

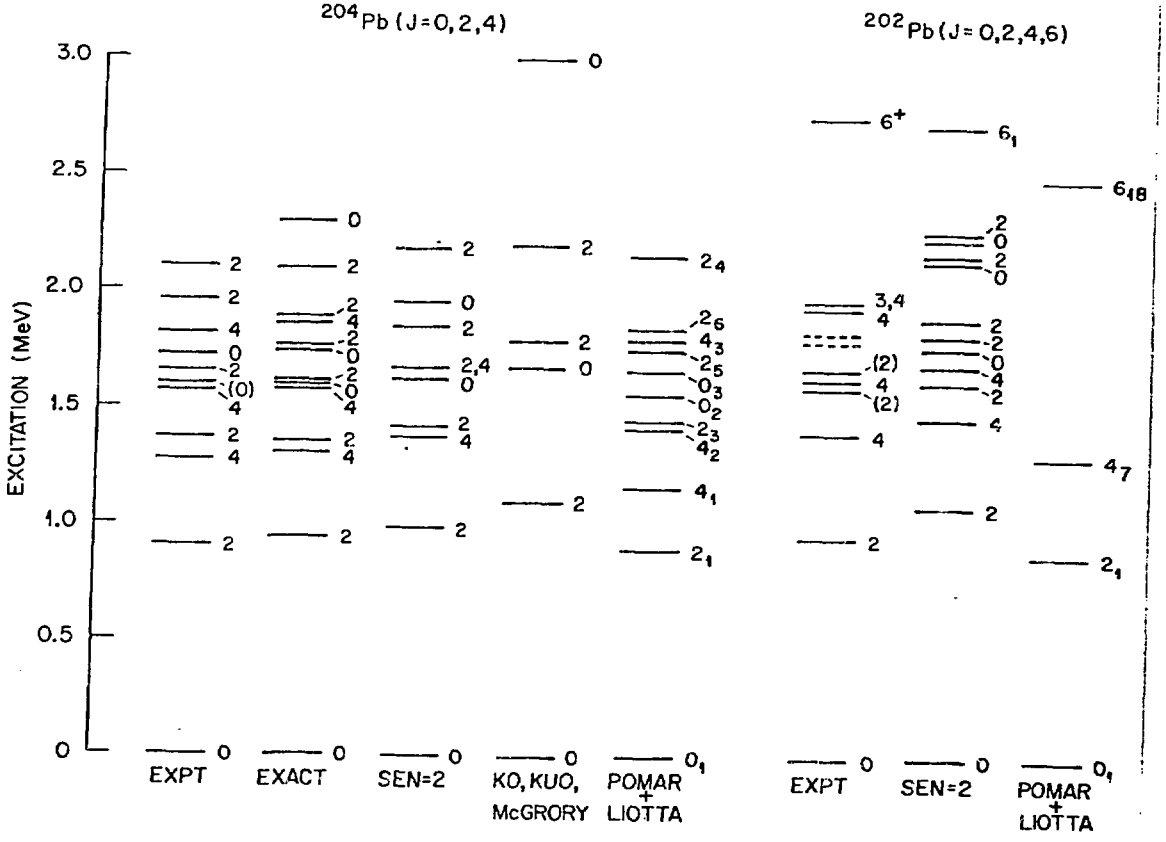

Figure 2 : Observed[13] and calculated spectra of ^{204}Pb and ^{202}Pb. The meanings of labels on spectra are given in the text.

knowledge of the actual spectrum. In the cluster calculations, the problem of too many low-lying states is much more apparent. There are seven $J=4^+$ states below the first $J=4^+$ state in experiment and in the seniority-2 calculation, and there are eighteen $J=6^+$ states below the first observed $J=6^+$ state. Thus, on the basis of published results, the cluster calculation is not as good as the simple seniority truncation. In Fig. 3 the known spectra of $^{206,204,202,200}Pb$ are compared with the seniority-2 calculations. Most of the systematic features of the data are accurately reproduced by the calculations, i.e., the increase in excitation energy of the lowest $J=2^+$ and 4^+ states in $^{204,202,200}Pb$, the sudden shift in the relative position of 0_2^+ and 3_1^+ states between ^{206}Pb and ^{204}Pb, and the sudden shift in the position of the lowest $J=9^-$ state between ^{206}Pb and ^{204}Pb. These latter two shifts are direct reflections of the Pauli blocking effect, i.e., in ^{206}Pb the ground state is predominantly $p_{1/2}^{-2}$. The first $J=2^+$, 3^+ state of $(f_{5/2}^{-1},p_{1/2})$ and the lowest negative parity state are $(p_{1/2}^{-1},s_{1/2}^{-1})_{J=6^-,7^-}$. There is no $p_{3/2}^{-4}$ state, so ^{204}Pb ground state is $(p_{1/2}^{-2},f_{5/2}^{-2})$. There are $J=2^+$ and 4^+ states in these configurations below the $(p_{1/2}^{-1},f_{5/2}^{-2})$. Then the lowest negative parity states are $(p_{1/2}^{-2},f_{5/2}^{-1},i_{13/2}^{-1})_{J=4^-,9^-}$. Thus, these results are the most recent pieces of data on the good shell model nature of the lead isotopes. The only "discrepancy" is that there is a $J=5^-$ state moving down in energy from $^{206}Pb \rightarrow {}^{200}Pb$ in the experimental spectrum, and this feature is not in the calculation. This could be a piece of the collective $J=5^-$ state seen in ^{208}Pb, which state is outside our space.

These results suggest that in our studies of the n-p coupling effects, the best first approximation is to use the seniority-2 scheme for the lead isotopes. This is the procedure followed below.

4. WEAK COUPLING CALCULATION OF $^{205,203}Tl$, $^{205,204,202}Hg$

In this section we present and discuss the results of weak-coupling calculations of some Tl and Hg isotopes near the ^{208}Pb closed core. In Fig. 4, the results for ^{205}Tl and ^{205}Hg are shown. For each isotope, the first column shows the spectrum of states deduced from experiments. The second column shows the results[12] of diagonalization in the complete space, as published by Pomar and Liotta. The third column

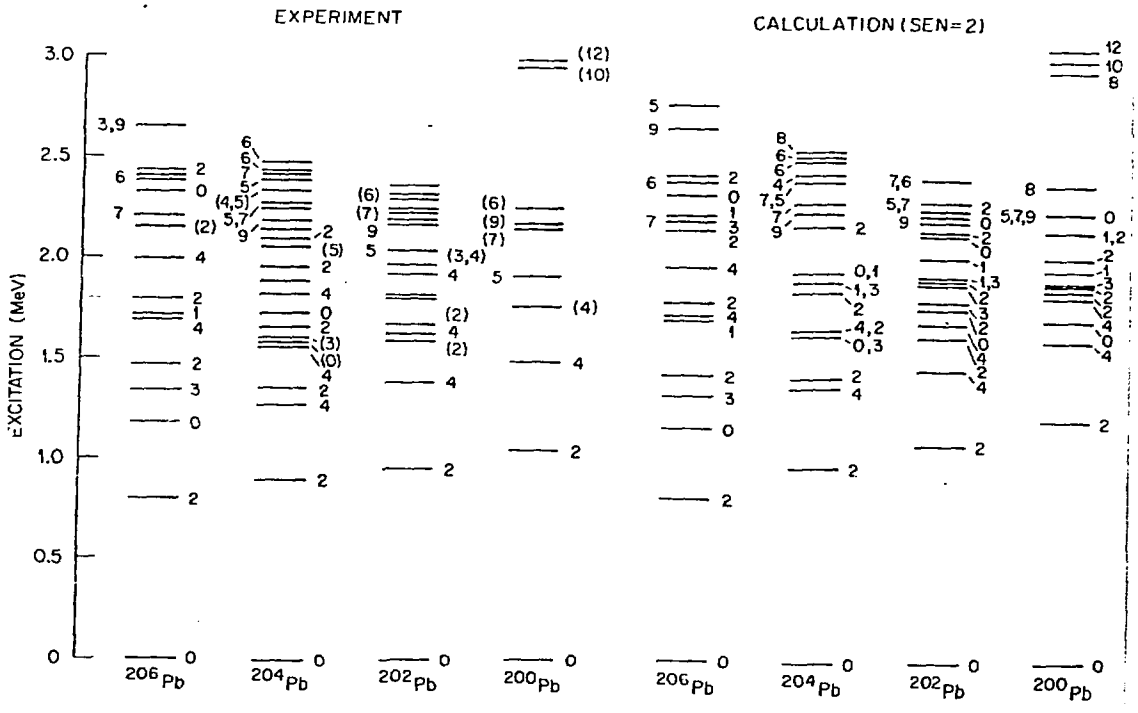

Figure 3 : Observed[13] and calculated spectra of $^{206,204,202,200}Pb$. Negative parity levels are labeled to the left of each spectra, positive parity levels to the right.

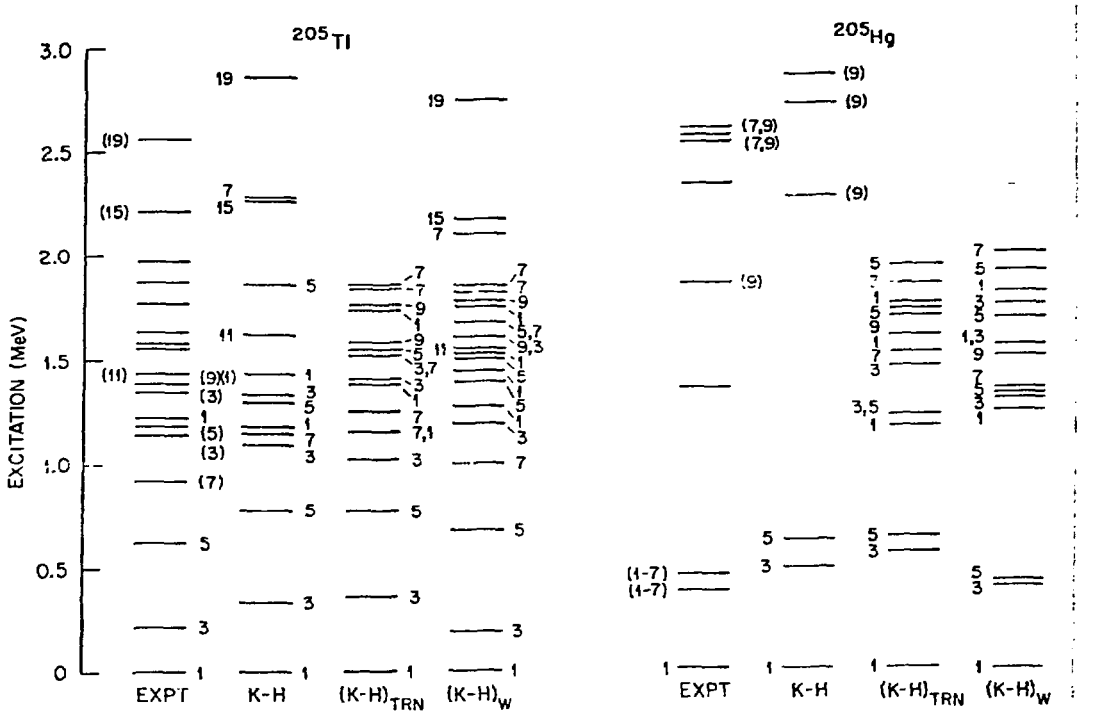

Figure 4 : Observed[13] *and calculated spectra of* ^{205}Tl, ^{205}Hg. *Negative parity levels labeled to the left of spectra, positive parity to the right.*

shows the results where the lowest 12 states in ^{206}Pb are included in the neutron cluster space. We see there is fair agreement with the known experimental data. In general, the excited states are somewhat too high in energy in the calculated spectrum (or, equivalently, the ground state is too low in energy), and there is an obvious inversion of the second J=3/2 and first J=7/2 states in ^{205}Tl. The truncated calculations differ in an inconsequential way from the full-space diagonalization results. Indeed, there is essential convergence when only the lowest five states in ^{206}Pb are included in the model space. This is shown in Fig. 5, where the results of a series of model space calculations of positive parity states in ^{205}Tl are shown. The number of neutron "clusters" in ^{206}Pb included in the model space are shown at the bottom of each spectrum, i.e., 1-3 means the first through the third states in ^{208}Pb are included in the model space. (In all cases, all five proton-hole states are included). When only the first two ^{208}Pb states are included, most of the low-lying spectrum of the "exact" calculation is present. Thus, the truncation, or weak coupling, approach seems to be a rather good approximation. The level-order discrepancy of the J=3/2 and J=7/2 states is the only obvious qualitative discrepancy. The two low-lying J=3/2 states are dominated by the states $(\pi\, s_{1/2}^{-1} \times (\nu^{-2}, J=2_1^+)$ and $(\pi\, d_{3/2}^{-1} \times (\nu^{-2}, J=0_1^+)$, in an obvious notation. These states are mixed only by the quadrupole-quadrupole component of the n-p force. Thus, a trivial renormalization of the n-p force was made by multiplying the Kuo-Herling n-p matrix elements by 0.8 and adding in the matrix element of the quadrupole-quadrupole force so as to roughly reproduce the splitting of the two low-lying $J=3/2^+$ states. Further, the $(s_{1/2}, p_{1/2})$ n-p hole interaction is weakened by 0.15 keV. This leads to the spectrum labeled $(K\text{-}H)_W$. In Fig. 4 $(K\text{-}H)_{TRN}$ and $(K\text{-}H)_W$ are calculations in the same model space. The $(K\text{-}H)_W$ interaction leads to an overall quantitative improvement in the theory-experiment agreement for ^{205}Tl and for ^{205}Hg. Thus, to the extent there is experimental data on spins and excitation energies, the simple calculations here reproduce experiment.

The calculated results for ^{203}Tl are shown in Fig. 6, where the calculated ^{203}Tl spectra result from coupling the single proton-hole states to all the ^{204}Pb states shown in the rightmost column. For the calculation $(K\text{-}H)_{TRN}$, only positive-parity levels are calculated, and above ~ 1.8 MeV excitation energy, only the lowest 11/2 and 17/2 levels are shown. The overall results are not very sensitive to the

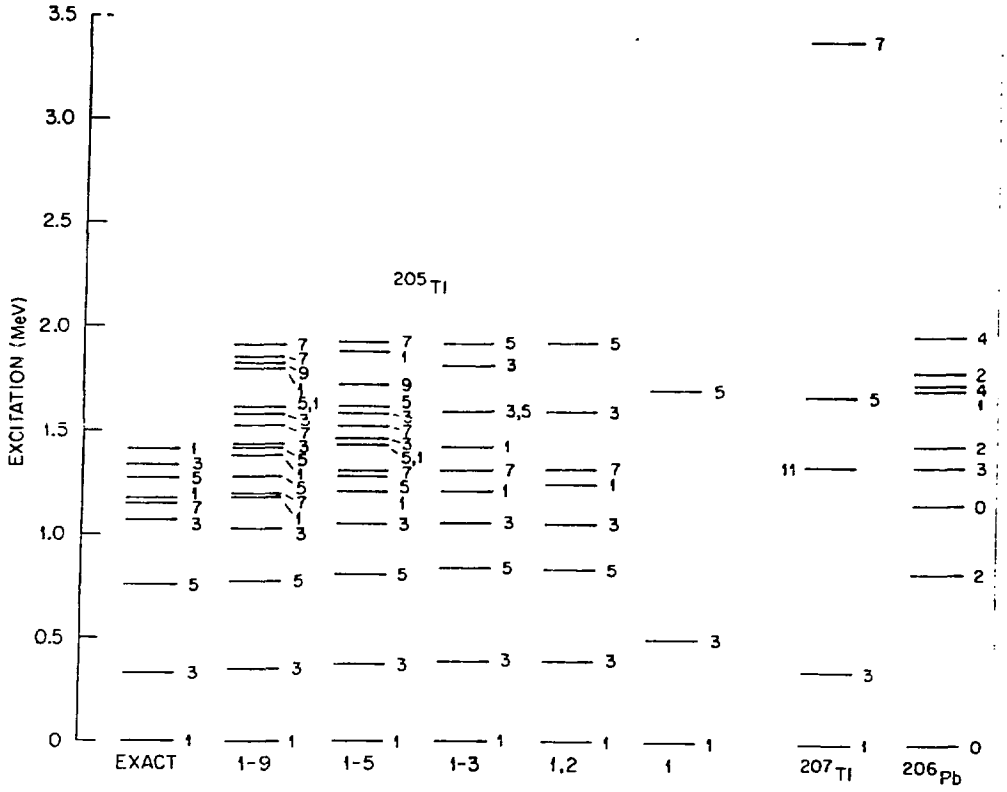

Figure 5 : Weak-coupling calculation of ^{205}Tl. Spectra labeled exact are from Ref. 12. The numbers under the remaining spectra label which states in ^{206}Pb are included in the weak-coupling space. The spectra labeled ^{207}Tl and ^{206}Pb should be "cluster" spectra.

differences in the two interactions. In both cases, the low-lying spectrum is too expanded. If one "mentally squeezes" the calculated spectrum, there is reasonable agreement between theory and experiment. In the calculations, the calculated eigenvalues of ^{204}Pb are used. These are from 50-100 keV too high with respect to known states in ^{204}Pb, and this accounts for some of the theory-experiment discrepancy in ^{203}Tl.

Finally, in Fig. 7 the results for ^{204}Hg and ^{202}Hg are shown. In this case, all states in ^{206}Hg below 2 MeV excitation energy are coupled to all states below 2.0 MeV in ^{206,204}Pb, respectively.

The calculations are only shown for one interaction, $(K\text{-}H)_N$ in ^{202}Hg. There is little data on ^{204}Hg. The calculation looks too expanded, *vis-a-vis* experiment, but there could be reasonable agreement. For ^{202}Hg, the picture is not satisfactory. The calculated spectrum is significantly expanded as compared to experiment. Again, a compressed spectrum bears some relationship to the experiment.

A number of these calculations have been repeated in various truncated bases. These other calculations suggest that the results shown here are probably fairly close to the results of exact diagonalizations (i.e., the truncation effects are small), although this must remain an unanswered question. If it is assumed these are more or less converged results, then a possible conclusion is that the n-p interaction used here is not accurate enough to make such calculations useful spectroscopic tools. One must look for simple renormalizations of the n-p interaction which give better results for these simple systems before one can push the calculations further away from the closed shell with any confidence.

5. SUMMARY

A weak-coupling approach to calculations of spectroscopic properties of nuclei near ^{208}Pb

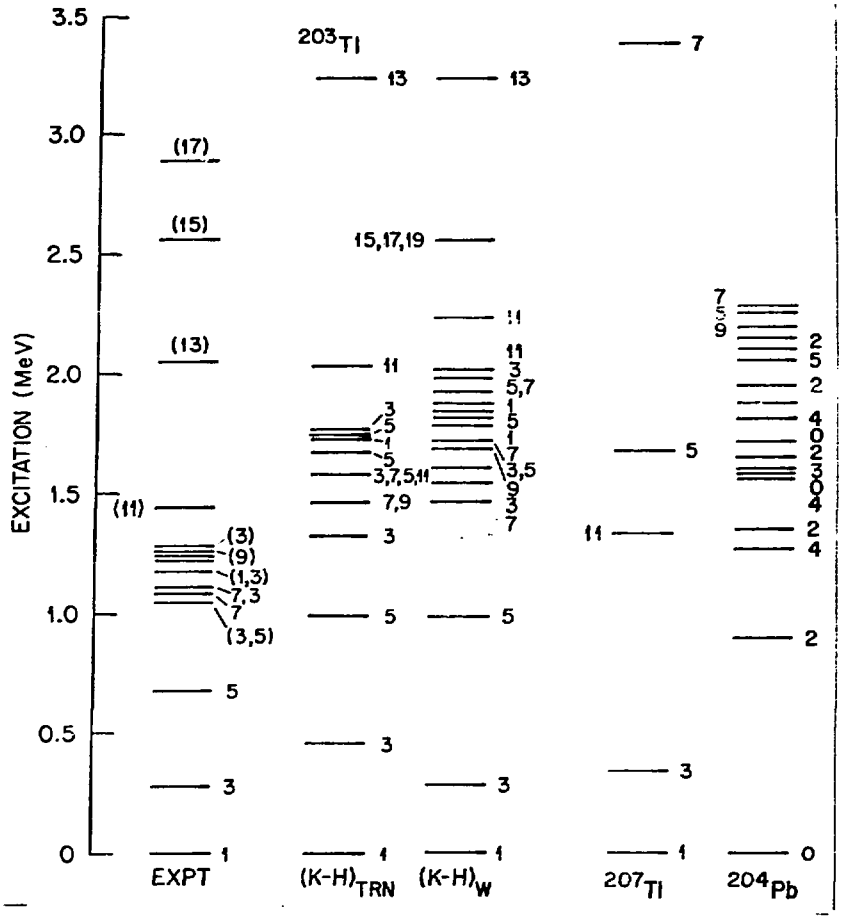

Figure 6 : Observed[13] and calculated spectra of ^{203}Tl. The weak coupling space includes all positive-parity states in the ^{204}Pb spectra shown in the rightmost column, positive-parity states are labeled on the right of the spectra.

has been discussed. The building blocks of the scheme are the eigenstates of the neutron-hole Pb isotopes and of the proton-hole system ^{207}Tl and ^{206}Hg. It is suggested that a simple "generalized" seniority-two calculation is the best truncation scheme for the identical-hole nuclei here as compared to potentially more powerful cluster schemes. The agreement of calculated levels with experiment is fair for the one-hole, two-hole systems ^{205}Tl and ^{205}Hg, but the agreement deteriorates for the larger systems. Studies of the results as a function of expanding bases spaces suggest that the weak coupling cluster approach used here is useful, i.e. only a few states at excitations ≤ 2 MeV are needed to reproduce more expanded space calculations. There is need for an improved n-p hole-hole interaction before the calculations can be extended to larger systems.

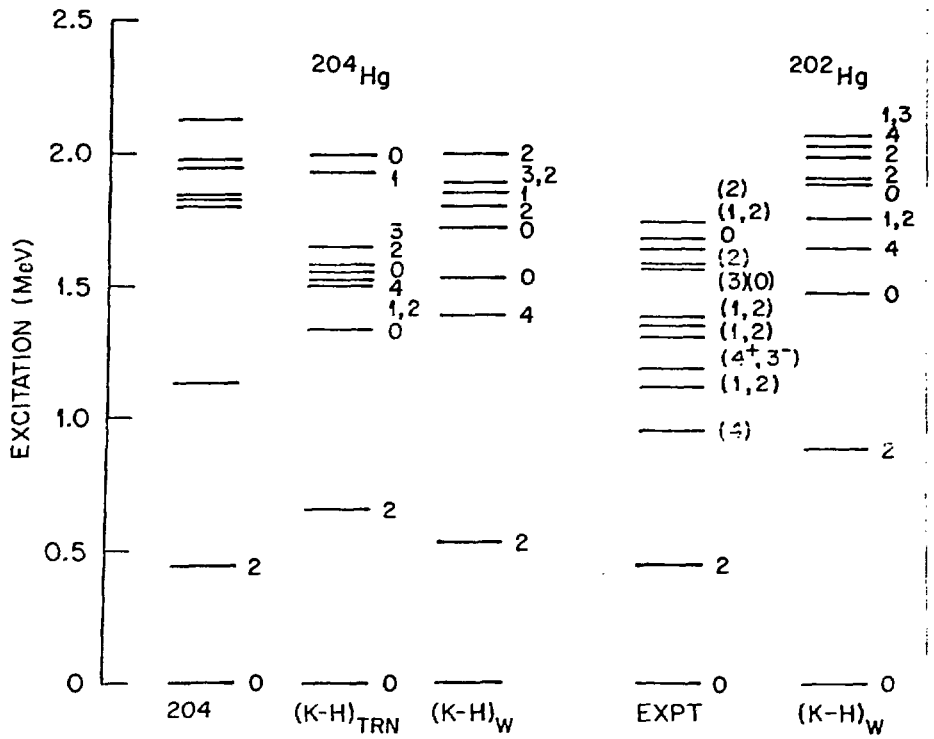

Figure 7 : Observed[13] and calculated spectra of states in ^{204,202}Hg. The weak coupling bases include all positive-parity states below 2.0 MeV excitation in the relevant proton and neutron systems.

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