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SHELL MODEL CALCULATIONS
FOR THE MASS 18 NUCLEI IN THE SD-SHELL

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1 Introduction

The basic input to a nuclear shell model calculation consists of a set of single particle energies and two body interaction matrix elements. There are two extreme approaches to generating this input. The first approach is to try and calculate the form of the operators from a theory based either on a perturbation approach, eg. the Brueckner-Hartree-Fock theory [1], or on some form of variational technique based upon a coupled cluster expansion [2, 3]. The second approach assumes that the matrix elements are considered merely as free parameters to be adjusted to fit the data on a number of neighbouring nuclei. This is exemplified by the work of Cohen and Kurath [4] and Wildenthal and his collaborators, Freedom and Wildenthal [5] (to be designated PW), Chung [6] and Chung et al [7] (to be designated CW) and Wildenthal [8]. Where the interaction of Cohen and Kurath was generated for the p-shell nuclei with $5 \leq A \leq 15$, the PW interaction was designed for the lighter region of the sd-shell with $17 \leq A \leq 22$, the work of CW ended with two A-independent hamiltonians one for the lower half of the sd-shell with $17 \leq A \leq 28$ (to be designated CWP) and the other for the upper half of the sd-shell with $28 \leq A \leq 39$ (to be designated CWH) and finally Wildenthal has postulated a simple mass dependence for the matrix elements,

$$ME(A)/ME(18) = (18/A)^{0.3} \quad (1)$$

from which a moderately successful description of all sd-shell nuclei can be obtained.

Irvine et al [9] generated a simple mass dependent effective interaction by folding a hamiltonian (for the rest frame of the nucleus) based on a good phenomenological bare nucleon-nucleon interaction (the Reid soft-core potential [10]) with a simple set of two body correlation functions. This interaction gave a better description of all the p-shell nuclei than that of Cohen and Kurath besides making excellent predictions for the absolute binding energies of all nuclei in this region. Yazici and Irvine [11] repeated this approach for the low mass sd-shell nuclei and, without adjusting a single parameter, demonstrated that their effective interaction matrix elements were in astonishing agreement with PW. Finally, we [12] extended the

work of Yazici and Irvine to the whole sd-shell and demonstrated that the 35 off-diagonal matrix elements of our interaction show no mass dependence and are in astonishing agreement with the fitted potentials of PW and CWP in the lower half of the sd-shell and with CWH in the upper half of the sd-shell while the 28 diagonal matrix elements can be brought into the same high level of agreement with the fitted matrix elements throughout the shell by a single, mass dependent energy shift. There was, in any case, an ambiguity in the choice of diagonal matrix elements connected with the choice of single particle energies. However, it was seen that our shifted diagonal matrix elements show a mass dependence very similar to that postulated by Wildenthal. In present work we shall examine our effective interaction matrix elements [12] and use it to determine the binding energies and energy spectra for the mass $A = 18$ nuclei with $T = 0$ and 1. The results of this shell model calculation will be compared with experiment [13] and with that obtained using Wildenthal's matrix elements.

2 Formalism

Our approach [12] to the problem of effective operators for shell model calculations involved two stages. In the first stage the bare operator must be formulated in the rest frame of the nucleus and can be written as

$$\hat{H} = \sum_{i>j} \left(p_{ij}^2/M(A) + V_{ij} \right) \quad (2)$$

where p_{ij} is the relative momentum $(1/\sqrt{2})(p_i - p_j)$, $M(A) = Am$ is the total mass of the nucleus and V_{ij} is taken to be the Reid soft-core potential. The second stage is to assume a set of trial variational wave functions

$$\Psi_J = F\Phi_J \quad (3)$$

where the Φ_J are the usual shell model basis states and F is a correlation function designed to accommodate those correlations which cannot be described by the shell model configuration mixing. A complete set of effective shell model operators is then defined by

$$O_{eff} = F^+ \hat{O} F \quad (4)$$

This in general is a many-body operator and it would be highly impractical to work thus it is usual to make a cluster expansion of O_{eff} to obtain a set of two body

effective operators $O_{eff}^{(2)}$. In the case of the operator of equation (2)

$$H_{eff}^{(2)} = F_2^+ \hat{H} F_2 \equiv \sum_{\lambda, i>j} f_{ij}^\lambda \left(p_{ij}^2/M(A) + V_{ij} \right) f_{ij}^\lambda \quad (5)$$

where F_2 are two body correlation operators and λ is summed over two body channels.

From studies of the nuclear matter saturation problem [3] it is clear that the correlation operators must take three features into account:-

(a) The short-range exclusion effect produced by the repulsive core of the bare N-N interaction. The core has an extremely short range ($\sim 0.4fm$) and the wound that it induces in the nuclear wave function is a property of the potential rather than the particular environment that the nucleon finds itself in. Thus if f_{ij}^λ is restricted to describing this short-range effect, leaving the shell model configuration mixing to account for longer-range correlations, two bonuses can be gained. Being short-ranged, any cluster expansion will rapidly converge and the two body approximation for $H_{eff}^{(2)}$ of equation (5) can be justified. Also the wound will be independent of mass, i.e. of the nucleus being considered.

(b) The strong correlations induced by the tensor force component in V_{ij} . These correlations are of longer range and may be expected to exhibit mass dependence.

(c) The effect of short-range $N^*(1232)$ isobar excitations. These correlations take us out of the nucleon space described by the Reid interaction but are essential if the nucleus is to have satisfactory saturation properties. However, the effect of isobar admixtures is small at normal nuclear densities and is only required at higher densities to remove the Coester line paradox. Thus we can, for energy level calculations, ignore this feature as an approximation.

Irvine et al [9] introduced the simple parametrization

$$f_{ij}^\lambda = f(r_{ij}) \left(1 + \alpha^\lambda(A) S_{ij} \right) \quad (6)$$

where $f(r_{ij})$ has the form

$$f(r_{ij}) = 1 - \exp[-\beta(r_{ij} - r_c)^2] \quad (7)$$

with $r_c = 0.25fm$ and $\beta = 25fm^{-2}$ and represents the short-range repulsion of (a). S_{ij} is the usual tensor operator and the strength of tensor correlations of (b) is measured by $\alpha^\lambda(A)$, $\alpha^\lambda(A) \equiv 0$ when $\lambda \neq {}^3S_1 - {}^3D_1$. We shall hereafter drop the label λ . The magnitude of $\alpha(A)$ was determined [9] by fitting it to the ground state

binding energies of ${}^4\text{He}$ and ${}^{16}\text{O}$ calculated in the closed shell approximation with oscillator wave functions chosen to give the correct root mean square radii, and to a Hartree-Fock calculation for nuclear matter. The results was a monotonically decreasing function with $\alpha(4) = 0.1, \alpha(16) = 0.08$ and $\alpha(\infty) = 0.06$. In the p-shell analysis the interpolation between $A = 4$ and $A = 16$ was made by fitting the ground state binding energy of the most stable isobar for each value of A .

Using the effective interaction of equation (5) with the correlation functions of equations (6) and (7) we have a mass dependent two body interaction, containing no free parameters with which to perform large basis shell model calculations.

3 Results and discussions

In calculating the two body matrix elements for a given mass number A there remain two parameters to be chosen namely: the oscillator parameter and the strength of the tensor correlations α . It was seen [12] that large values of α and $\hbar\omega$ (eg. $\alpha = 0.085, \hbar\omega = 14$ MeV) are more appropriate to the beginning of the sd-shell while smaller values of α and $\hbar\omega$ (eg. $\alpha = 0.07, \hbar\omega = 10$) give better fits to the upper end of the shell. An acceptable fit to the whole shell was obtained with 'average' values of $\alpha = 0.08$ and $\hbar\omega = 11$ MeV, provided we used the mass dependent energy shift Δ_{sd} given in ref. [12].

A set of two body matrix elements of our interaction applicable throughout the whole sd-shell is presented in table (1) of ref. [12]. In order to test these matrix elements, shell model calculations are performed for two nucleons in the sd-shell. The single particle energies used with the two body matrix elements of our interaction are the experimental energies [16] from ${}^{17}\text{O}$, namely: $-4.15, -3.28$ and 0.93 MeV for $j = 5/2, 1/2$ and $3/2$ respectively. Results for the energy spectra obtained for the mass $A = 18$ with $T = 0$ and 1 are displayed in figures 1 and 2 respectively. In these figures, the energy spectra of our calculation are compared with experiment and with that obtained when using Wildenthal's empirical matrix elements [8].

It is evident from above figures that a number of the low-lying experimental levels are not reproduced by our calculation. This is mainly because of the model space which we have chosen for our calculation. Our model space consists of a closed ${}^{16}\text{O}$ core with two active valence nucleons confined in the sd-shell. Thus our calculated levels for ${}^{18}\text{F}$ and ${}^{18}\text{O}$ are those whose wave functions are predominantly of $2p0h$

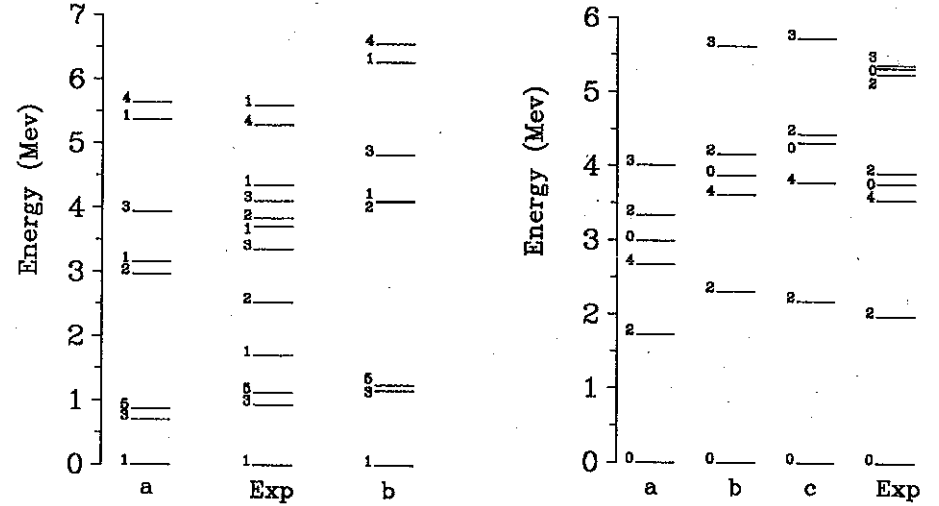


Fig. 1. Positive-parity energy spectra for ${}^{18}\text{F}$ with ($T = 0$). The calculated spectrum (a) is compared with experiment (Exp) and with that obtained using Wildenthal's matrix elements (b).

Fig. 2. Positive-parity energy spectra for ${}^{18}\text{O}$ with ($T = 1$). The calculated spectrum (a) is compared with experiment (Exp) and with that obtained using Wildenthal's matrix elements (c). In spectrum (b) we use Wildenthal's diagonal matrix elements but with our off-diagonal matrix elements together with experimental single particle energies.

(two-particle-no-hole) nature. In order to account for those observed levels of $A = 18$ nuclei we have to consider the mixing of the $(sd)^2$ configurations with deformed $4p2h$ states. Hence it is not unexpected that these states are not reproduced well by our calculation nor by Wildenthal's calculation which is also based on a closed ${}^{16}\text{O}$ core model space.

The energy spectra of ${}^{18}\text{F}$ nucleus is presented in figure 1, which have been rather extensively studied in ref. [14, 15]. We note that Wildenthal, spectrum (b), included the lowest six states in his fit as these states are generally believed to be predominantly of $2p0h$ nature. Our calculation, spectrum (a), has given these six levels and are well reproduced in comparison with experiment and with that

obtained by using Wildenthal's matrix elements. It is seen that our interaction gives less binding to this nucleus than experiment. Hence the difference between the ground state energies obtained from experiment and our interaction is about -0.6 MeV.

We now turn to the energy spectra of ^{18}O nucleus which is presented in figure 2. The experimental 3.63 MeV 0^+ , 5.26 MeV 2^+ and 7.12 MeV 4^+ (where the experimental 4^+ state is not shown in figure 2) of ^{18}O are well known to be members of a $4p2h$ band. Therefore, these states are not reproduced well by our calculation, spectrum (a). We note that Wildenthal, spectrum (c), included only the lowest 0^+ , 1.98 MeV 2^+ and 3.55 MeV 4^+ states in his fit. This is clearly a reasonable thing to do as these states are well known to be of $2p0h$ nature. It is obvious from the calculated spectrum that the level sequence of the low-lying states is correctly reproduced besides the lowest 2^+ state is in good agreement with experiment. The lowest 4^+ and the second 2^+ states are lower than the experimental results by about 0.8 and 0.6 MeV, respectively. The comparison between the spectra (a) and (c) gives an indication that Wildenthal's interaction is stronger than our interaction. This is demonstrated even more clearly by looking at the energies of the system with two valence nucleons relative to the ground state energy of the ^{16}O core. For the ground state of ^{18}O nucleus we obtain for this energy -11.37 and -12.17 MeV using ours and Wildenthal's interactions respectively. Comparing this energy with the experimental value -12.18 MeV, we see that our interaction gives less binding than experiment or than Wildenthal's interaction by about -0.8 MeV. As we have mentioned before that our diagonal matrix elements have been shifted throughout the shell by a single mass dependent energy shift [12]. Such a shift would not show up in the spectroscopy of any set of isobars but would simply change the relative binding energies of different isobaric sets of states. Therefore, an improvement can be obtained for the ground state energies if we vary the energy shift within the limits set that would not impair our quality of fit to the fitted matrix elements of CW interaction by more than $\Delta\chi = 0.005$ about its optimum values. Thus, for example, increasing the shift by -0.3 MeV, we see that the differences between the ground state energies obtained from experiment and our interaction are now reduced to about -0.3 and -0.5 MeV for ^{18}F and ^{18}O nuclei respectively. Spectrum (a), of figure 2, can usefully be compared with spectrum (b) where Wildenthal's diagonal matrix elements are used but with our off-diagonal matrix elements. The differences are then due entirely to defects in

the diagonal matrix elements and these are clearly quite pronounced. In spectrum (b), we obtain energy -12.22 MeV for the ground state of ^{18}O which is very close to the experimental value. Finally, we would like to point out that Wildenthal's interaction gives results are in better agreement with experiment than ours or any body else, with the exception of PW or CW interactions because of their limited mass range of applicability.

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