J. Nig. Ass. Math. Phys.
Vol. 6 (2002)

MISSING IDEAS: SELF-CONSISTENCY PROBLEM IN THE DERIVATION OF THE ONE- ANDTWO- BODY EFFECTIVE INTERACTIONS FOR *SD* SHELL-MODEL CALCULATIONS

J.O. FIASE AND L.K. SHARMA
Department of Physics, University of Botswana,
Private Bag 0022, Gaborone
Email: fiasejo@mopipi.ub.bw

The input data to the shell model for nuclear energy level calculations consists of a set of single-particle energies on the one hand and a set of two-body matrix-elements on the other. The single-particle energies are usually extracted from experimental data, whereas, various empirical and theoretic techniques are used in the determination of the two-body matrix elements. Thus there is no self-consistent approach in the determination of these quantities. Using the method of lowest order constrained variational approach (LOCV) with a set of two-body correlation operators, we have calculated a set of single-particle energies together with a set of two-body matrix elements self-consistently. We have used the results to calculate the energy spectra of ^{19}O and ^{19}F nuclei and have found that the calculated spectra are rather compressed. However, on keeping our single-particle energies fixed at their calculated values and replacing some of our calculated two-body matrix elements with the Chung-Wildenthal empirically fitted two-body interaction, we have found a reasonable agreement with experiment.

These results demonstrate that shell-model calculations can be done quite successfully with the single-particle energies derived from the interaction but that there is a self-consistency problem in determining the nuclear spectra entirely from the microscopic theory.

1 INTRODUCTION

For sometime now, the shell model has come to play a major role in the understanding of nuclear structure. The combination of this model with the experimental techniques has enabled us to understand the building blocks on which nature is based on at least at the level of protons and neutrons. From this we, of course, make the assumption that the internal degrees of freedom of both protons and neutrons are not excited. Even with the aforesaid assumption the problem is still a formidable one because this is a many-body problem and the dimensions of the Hamiltonian for an A-body system, where A> 3 is not easily tractable. This means that further assumptions have still to be made. One assumption to be made is to remember that the structure of nuclei with magic numbers such as ^{16}O are particularly stable. One can then assume that in defining the Hamiltonian for an A-body system, the part of the Hamiltonian that constitute the magic core should remain inactive and should simply contribute a constant energy. We are then left with the model space with which to do our

shell-model calculations by further assuming that there is no overlap between the core states and the states outside the core, the so-called valence states. The Hamiltonian therefore splits into the core and the valence space and as we shall show in the following that the new Hamiltonian is still able to account for the neglected configurations from the core. This new Hamiltonian is better described by the term 'effective interaction.' In such calculations, the energy of a state having an angular momentum J, isospin T is found by diagonalising the Hamiltonian matrix:

$$< \mathrm{H} >_{JT} = E_0 + \sum_i \mathrm{e}_i + \sum_{i>j,k>l} < ij|V_{eff}|kl >_{\mathrm{JT}}, \qquad (1)$$

where in this equation, E_0 is the binding energy of the closed core which is taken to have a constant value. For example, for the sd shell-model calculations (A=16 - 40), ^{16}O is taken to be a closed-shell core and this has a constant value of (-127.62) MeV while the e_i are the single- particle energies. These are usually experimentally determined from the (d,p) reaction of ^{16}O(d,p)^{17}O. Here the single-particle states are clearly seen in the ^{17}O spectrum [1] with their corresponding energies as shown in Fig. 1 (a). The last term in equation (1) represents the two-body matrix elements of the residual interaction between the valence orbits i, j, k and l.

In order to determine the last term in equation (1), various empirical and theoretical techniques are used [2,3]. The empirical approach treats all the single-particle energies together with the two-body matrix elements as free parameters. These are adjusted until they fit the experimental spectrum. Several groups have followed this approach with a high degree of success [2,4]. Yet the microscopic approach demands that these quantities have some theoretical basis. This approach studied by many authors [5,6], attempts to explain all the experimental properties of nuclei with microscopic theory.

While the energy spectra of various nuclei has been extensively studied in terms of the single-particle energies extracted from experiment and various two-body matrix elements [7], the spectra of nuclei in terms of the single-particle energies derived microscopically has received scanty attention. Because of the difficulty to microscopically determine the single-particle energies accurately, most researchers prefer to extract them from experiment.

The method of lowest order constrained variational technique(LOCV) which we outline below is a very powerful method of calculating both the single-particle energies and the two-body matrix elements, very accurately. This method rivals an alternative method known as the G-matrix technique [3]. In this method we have devised a way of dealing with the repulsive core of the N-N interactions by introducing two-body correlation functions in the wave function. As will be shown, this enables us to calculate two-body matrix elements in a simple way with an accuracy of the order of the empirical interactions [5]. Recently [8], we have used the same method to derive a set of mass-dependent single-particle energies for sd shell-model calculations. Our aim in this paper is to use the set of single-particle energies discussed in ref. [8] in combination with our two-body

effective interactions and also the Chung- Wildenthal [4] empirically determined two-body matrix elements to calculate the energy spectra of ^{19}O and ^{19}F nuclei. This approach differs from other calculations, where the single-particle energies are usually extracted from experiment. Our aim is to emphasise by showing that the shell-model calculations can be done quite successfully with single-particle energies derived from theory. The rest of the paper is organised as follows: In section 2, we give an outline of the LOCV method used. In section 3, we give the results of our calculated energy spectra and compare them with experiment and that of the other works on ^{19}O and ^{19}F nuclei. Section 4 is devoted to the summary and conclusion of the paper.

2 THE LOWEST ORDER CONSTRAINED VARITATIONAL METHOD (LOCV)

In this section we give a summary of the LOCV approach discussed in Refs. [5,8] for evaluating the two-body effective interactions. The non-relativistic Hamiltonian for an A-nucleon system is approximated as:

$$H_0 = \sum_i p^2 / 2m + \sum_{i>j} V_N(ij), \tag{2}$$

where $V_N(ij)$ is the NN potential and m is the nucleon mass.

Since the NN potential of eq. (2) is known to have a large repulsive component which makes it difficult to apply the direct Hartree-Fock formulae. The Hartree-Fock wave function:

$$\Phi = (A!)^{-1/2} \det \phi_i(\vec{r}_j) \tag{3}$$

must be correlated in the form:

$$\Psi = F\Phi, \tag{4}$$

where the ϕ_i are the single-particle basis functions and F is a symmetric product of two-body correlation functions [9]:

$$F = S\prod_{ij} f_{ij}. \tag{5}$$

Such correlations were formulated in order to accommodate the effect of the strong repulsive component of the NN interaction. In this equation, S is the symmetrizer operator. Furthermore, we require that the Hamiltonian be formulated in the rest-frame of the nucleus. This is achieved through a unitary transformation [10]:

$$H_0 \rightarrow \overline{H} = H - P^2 / 2M = \sum_{i>j} (p_{ij}^{\ 2} / M + V_N(ij)), \tag{6}$$

where $M = m_N A$ is the total mass of the nucleus, $P^2/2M$ is the translational kinetic energy of the centre of mass of the nucleus, $\vec{p}_{ij} = 1/\sqrt{2}(\vec{p}_i - \vec{p}_j)$ is the relative momentum of the two interacting

particles. For the NN potential, $V_{\cdot}(ij)$ hereafter denoted as V_{ij} we have used the Reid [11] soft-core potential.

Owing to the dimensionality problem mentioned above, we chose a model space where only the two-body effective interactions are important, since working with the full shell-model Hilbert space is not possible. The justification for this approach has been fully explained in [10]. The two-body effective interactions have therefore been formulated in the form (Irvine [10]):

$$H_{eff}^{(2)} = \sum_{i>j}(f_2(ij)(p_{ij}^2/M + V_{ij})f_2(ij)), \tag{7}$$

where $f_2(ij)$ are the two-body correlation operators. In previous calculations [5] it was required that the two-body correlation functions should take on the features of the chosen potential used, which in our calculation was the Reid [11] soft-core potential. The Reid [11] potential has the form

$$V_{ij} = \sum_k V_{ij}^k \tag{8}$$

where k is a reaction channel which has the central, spin-orbit and tensor components. In a similar manner we have expanded the correlation operators as:

$$f_2(ij) = \sum_k f_{ij}^k, \tag{9}$$

where

$$f_{ij}^k = f_c^k(r_{ij}) + f_{LS}^k(r_{ij})\vec{L}.\vec{S} + f_T^k(r_{ij})S_{ij}. \tag{10}$$

Earlier calculations on nuclear matter and finite nuclei [10] have shown that only central and tensor correlations are more significant. This permits us to parameterize the two-body correlation functions in these channels in the form [5]:

$$f_2(ij) = 0, r_{ij} < r_c$$

$$f_2(ij) = (1 - e^{-\beta(r_{ij}-r_c)^2})(1 + \alpha^k S_{ij}), r_{ij} \geq r_c, \tag{11}$$

where $r_c = 0.25\,fm$ and $\beta = 25\,fm^{-2}$. The parameter α^k represents the strength of the tensor correlation and is non-zero only in the $^3S_1 - ^3D_1$ channel.

The two-body matrix elements of the effective Hamiltonian defined in eq. (7) were calculated in a harmonic oscillator basis. The general expression for evaluating the two-body matrix elements:

$$< (ab)JT \left| H_{eff}^{(2)} \right| (cd)JT >_{AS} \tag{12}$$

is reported in Refs. [3,8].

Furthermore, one can calculate the single-particle energies ε_i from the same interaction according to the equation [8]:

$$\varepsilon_i = \sum_{kJT} \frac{(2T+1)(2J+1)}{2(2l+1)} < (kl)JT \left| H_{eff}^{(2)} \right| (kl)JT >_{AS} . \qquad (13)$$

where in this equation the sum k, is limited to the core states and l to the valance space orbitals. Note that in our calculations of eqs. (12) and (13) there are only two free parameters. These are the oscillator size parameter and the strength of the tensor correlations α^k. We varied these to obtain the best set of the one- and two-body effective interactions to calculate the ^{19}O and ^{19}F spectra.

3. THE RESULTS

We now use the results of the two-body effective interactions defined in eq. (12) and the set of single-particle energies defined in eq. (13) calculated by the method of Ref. [8] for evaluating the energy spectra of ^{19}O and ^{19}F nuclei. The single-particle energies calculated by our method are shown in Fig. 1(b).

In Fig. 2(a), the calculated spectrum of ^{19}O using our interaction is presented together with the experimental spectrum [12] for the positive parity states of ^{19}O. For comparison, we also present the result of the shell-model calculation using the Chung-Wildenthal (CW) empirical effective interaction [4] which is best suited for this mass region of nuclei. We denote a state by J_i^{π} ; T where J is the total angular momentum of the two-particle system while T is their corresponding isospin. For the ^{19}O nuclei, only T=3/2 states are observed, so we have suppressed their labelling in the figure. From Fig. (2a) we see that our calculated energy spectrum is rather compressed when compared with the experimental energy spectrum. We have repeated the same procedure in Fig. (2b) but this time with the single-particle energies extracted from experiment, but this also provides the same result. Indeed, Kuo and co-workers [3] have made a similar observation with regard to forces with a strong tensor component to which the Reid [11] potential used here also belongs. Since our calculated spectra are compressed either with single-particle energies calculated from the interaction or with those extracted from experiment, we conclude that our problem resides in our calculated two-body matrix elements. We therefore decided to alter our two-body matrix elements by comparing them with their CW counterparts. Those matrix elements in our calculation that differed by more than 150 KeV from their CW counterparts were replaced by their CW values. In doing so we retained only 21 two-body matrix elements from the 63 Pauli-allowed two-body matrix elements in our calculation. The remaining 42 were therefore the CW empirical matrix elements. We kept the single-particle energies fixed at their calculated values.

In Fig. 3(a) we notice an impressive agreement with experiment. The first five experimental levels: $(5/2)_1^+$; 3/2, $(3/2)_1^+$; 3/2, $(1/2)_1^+$; 3/2, $(9/2)_1^+$; 3/2

and $(7/2)_1^-$; 3/2 at energies of 0.0, 0.096, 1.47, 2.37 and 2.78 MeV respectively are well reproduced at energies of 0.0, 0.21, 1.16, 2.45 and 2.66 MeV respectively using our single-particle energies calculated from the same interaction. When the single-particle energies from experiment are used adopting the same procedure, the same states are predicted at energies of 0.0, 0.14, 1.52, 2.30 and 2.80 MeV respectively as shown if Fig. 3(b). For a comparison, we have also calculated the same states using CW empirical effective interaction. This interaction puts these states at energies of 0.0, 0.29, 1.47, 2.48 and 2.96 MeV respectively. Thus, it can be conjectured that our calculated single-particle energies are capable of predicting at least the low-lying positive parity states of ^{19}O. Beyond the $(7/2)_1^-$; 3/2 state, there is no one-to-one comparison between our calculated spectrum and the experiment. This same problem is seen even with the CW interaction which has been fitted with the experimental data.

In Fig. 4, we repeat the same procedure as given in Fig. 3 for the calculated spectrum of ^{19}F and present also the experimental spectrum [12] of the positive parity states of ^{19}F nucleus. For the ^{19}F nuclei, only T=1/2 states are observed, so we have suppressed their labelling. In a similar manner to Fig. (3), we altered our two-body matrix elements by replacing those that differed by more than 150 KeV with the CW interaction by their CW counterparts while keeping the single-particle energies fixed at their calculated values. Here again for comparison we present the result of the shell-model calculation of the CW interaction. From Fig. 4, it can be seen that the first four experimental levels: $(1/2)_1^-$; 1/2, $(5/2)_1^+$; 1/2, $(3/2)_1^+$; 1/2 and $(9/2)_1^+$; 1/2 at energies of 0.0, 0.197, 1.55 and 2.78 MeV respectively are also well reproduced by our method in Fig. 4(a) when single-particle energies from our interaction are used. Here these states are predicted at 0.0, 0.17, 1.15 and 2.95 MeV respectively. However, if we use the single- particle energies extracted from experiment, these states are predicted at energies of 0.0, 0.02, 1.52 and 2.43 MeV respectively as shown in Fig 4(b). These may be compared with the prediction of the CW interaction which puts them at the energies of 0.0, 0.099, 1.699 and 2.81 MeV respectively. Beyond these energies we have a similar problem as was noticed in the ^{19}O case where we could not get a one-to-one correspondence between our calculated spectra and their experimental counterparts. This is also the case with the CW interaction.

4. SUMMARY AND CONCLUSION

In this paper we have carried out a shell-model study of the energy spectra of ^{19}O and ^{19}F nuclei. We have found that our two-body effective interactions and the single-particle energies alone are not capable of providing a good description of the energy spectra of these nuclei. We therefore substituted some of the matrix elements of our effective two-body interaction that differed by more than 150 KeV with their counterparts from the CW empirically fitted interaction, and repeated the energy spectra calculation while keeping our single-particle energies fixed at their calculated values. With this procedure, we found that the overall spectra for the low-lying states for both nuclei are in

excellent agreement with experiment as well as the results of other workers on these nuclei.

Though the calculation of nuclear energy spectra such as presented in this paper is not new, it should be noted that in most microscopic shell-model calculations, the set of two-body effective interactions are derived microscopically but the set of single -particle energies are extracted from experiment [1]. Our approach here has been to emphasise that the spectra of nuclei can be calculated with single-particle energies derived from theory. These calculations should still be regarded as a first-step calculations. Indeed we have neither considered the effect of core-excited states in our calculation nor have we extended our approach to include the delta resonances in nuclei which will require going over from the usual N-N sector to include the N-Δ sector. These are some of the reasons why our two-body matrix elements had to be substituted with their empirical counterparts in order to improve the spectra of the calculated nuclei.

We have also not considered electromagnetic properties of these nuclei in our calculations which are a stringent test for a successful shell-model calculation. Yet our modest attempt seems to be quite promising in predicting the low-lying energy levels of nuclei. In our next paper we intend to include the above aspects omitted here in our two-body effective interaction and thus extend our approach to other nuclei as well. Our ultimate aim is to be able to calculate the energy spectra and electromagnetic properties of nuclei very accurately in a self-consistent manner. This is a problem which no microscopic theory has been able to provide yet.

ACKNOWLEDGMENT

One of the author (JOF) wishes to thank Professor J.M. Irvine who introduced him to shell-model effective interactions. Computational work was done with the Glasgow shell-model code.

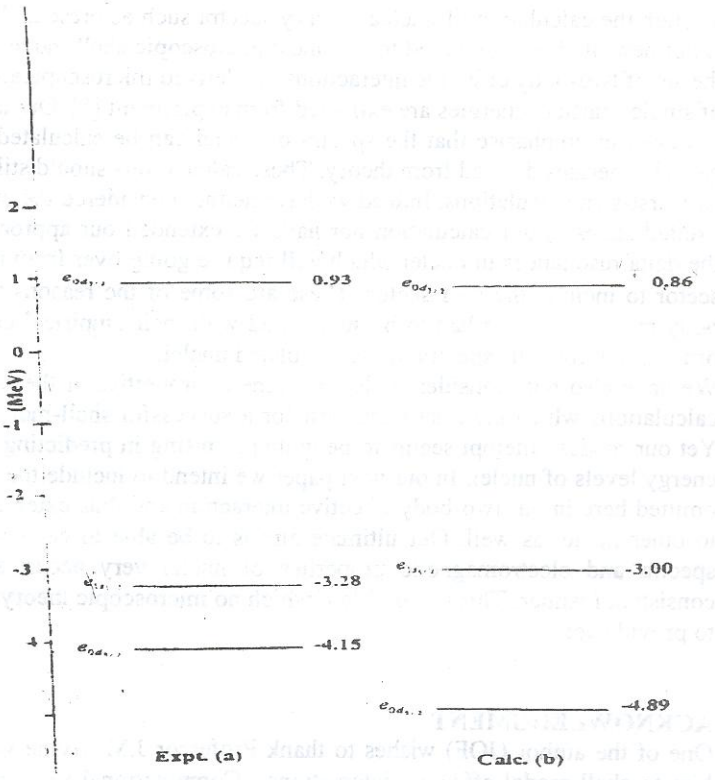

Fig. 1

Fig. 1 : Experimental and calculated Single particle energies in 17_0 used in the present work.

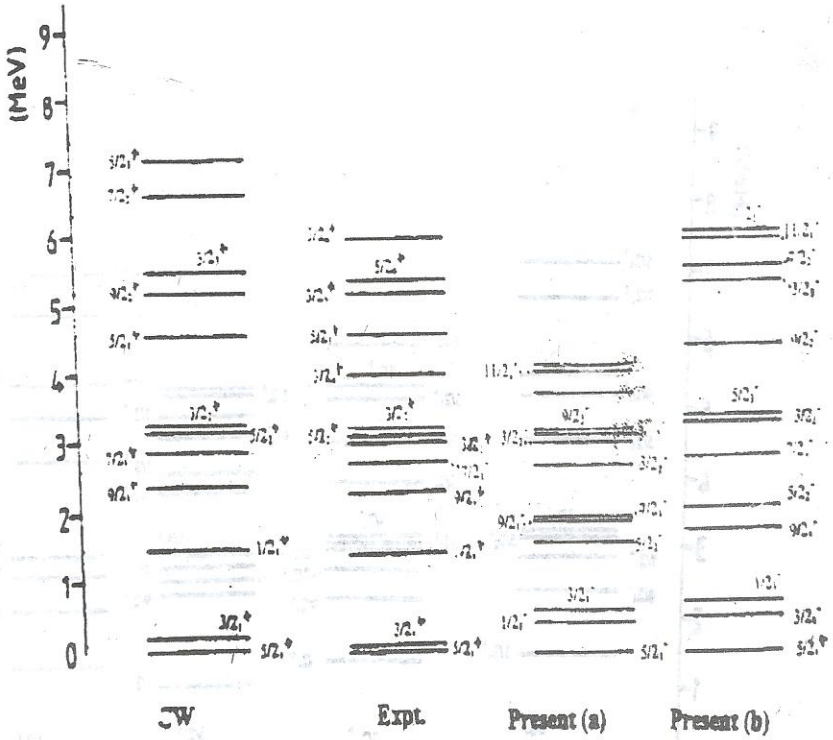

Fig. 2: Calculated energy spectra of ^{19}O nucleus compared with experiment and CW interaction. (a) is the result of the present calculation with single-particle energies derived from the interaction . (b) is the result of the present calculation with single-particle energies extracted from experiment. Notice, that our interaction gave spectra that is compressed either with single-particle energies from the interaction or those extracted from experiment.

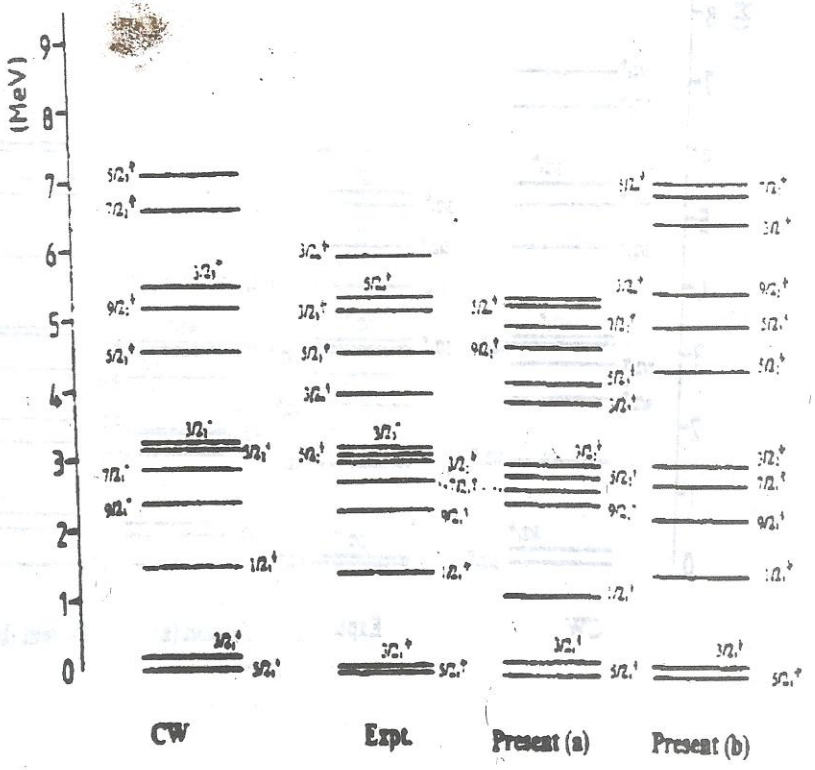

Fig. 3: Calculated energy spectra of ^{19}O nucleus compared with experiment and CW interaction. (a) is the result of the present calculation with single-particle energies derived from the interaction and two-body effective interactions as discussed in the text. (b) is the result of the present calculation with single-particle energies extracted from experiment and the two-body effective interactions as described in the text.

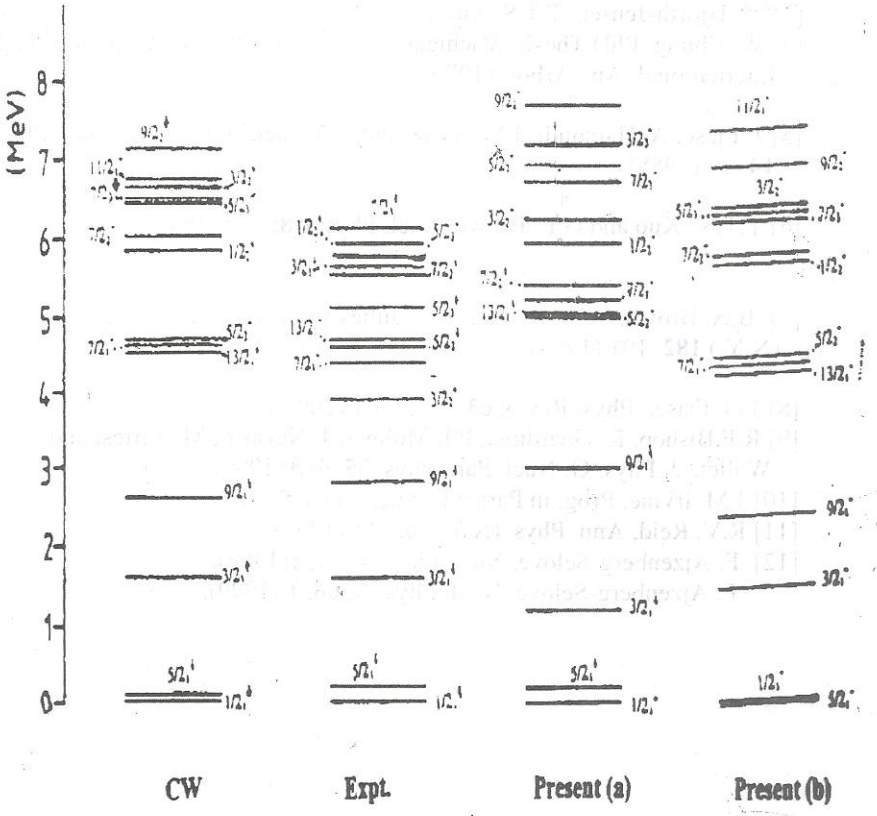

Fig. 4: Calculated energy spectra of ^{19}F nucleus compared with experiment and CW interaction. (a) is the result of the present calculation with single-particle energies derived from the interaction and two-body effective interactions as discussed in the text. (b) is the result of the present calculation with single-particle energies extracted from experiment and the two-body effective interactions as described in the text.