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Shell model in nuclei—a historical overview

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Abstract. The nuclear shell model is (over)viewed with examples from its early phase to its current status.

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1. Introduction

The first serious proposal for a shell-model in nuclei was made independently by Mayer (following a suggestion of Fermi) and by Haxel, Jensen and Suess (see Mayer and Jensen 1955). The underlying picture in the model is that each nucleon moves in an average potential which is created by its interaction with all the other nucleons in the nucleus and is identical for all nucleons. This simple single particle model has been remarkably successful in correlating a large amount of experimental data in nuclei.

It ought to be mentioned here that, prior to 1949 when the shell-model was proposed, the general view amongst physicists was that, for a complicated system like the nucleus, one had to invoke a liquid drop type model. This view was held very likely due to the successful application of the liquid drop model to nuclear binding energies (semi-empirical mass formula) by Weizsacker (1935) and Bethe (1936) and to fission problem by Bohr and Wheeler (1939). Thus, the success of the single particle shell model was a big surprise but it also provided theoretical nuclear physicists with a tremendous challenge: to attempt to explain the properties of nuclei in terms of an apparently simple shell model which must be deduced from a microscopic, quantum, many-body theory involving neutrons and protons (and perhaps mesons) and their mutual interactions.

Nearly forty years after the introduction of the shell-model the activity is still continuing and evolving. There has been much progress and many successes and as it appears not too many unresolved questions. It is important to realise that crucial to all these developments, has been the increasing availability of high quality data and high speed computer facilities.

We review here, partly in an historical manner, the shell-model and its development. The early work is discussed in §2 and the more recent work in §3. The last section contains some concluding remarks and the outlook for the future.

2. Shell model—The early phase

In a formal sense, the shell-model is a tool to solve the many-body problem for a nucleus consisting of A nucleons (N neutrons, Z protons, $A = N + Z$) and described by the Hamiltonian H

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j}^{A} V_{ij}. \tag{1}$$

Here the first term is the kinetic energy of the nucleons and the second term is the interaction (assumed to be two-body) between the nucleons. As is well-known this is an impossibly complicated problem to solve exactly. In order to simplify the problem one resorts to the idea of the average potential—i.e. H of (1) is rewritten as

$$\begin{aligned} H &= H_0 + H_1 \\ H_0 &= \sum_{i=1}^{A} \left(\frac{p_i^2}{2m} + U_i \right), \\ H_1 &= \sum_{i<j}^{A} V_{ij} - \sum_{i=1}^{A} U_i, \end{aligned} \tag{2}$$

where U_i is the average potential experienced by the ith nucleon.

There are various ways of proceeding further. One may from the known nucleon-nucleon interaction try to compute the average potential, using the Brueckner Hartree-Fock method. This would be theoretically the most satisfying approach, although there are uncertainties about the interaction, and the computations are involved. In their original work, Mayer and coworkers (see Mayer and Jensen 1955) followed a phenomenological approach and took for U the (central) harmonic oscillator potential together with a strong one body spin-orbit term—i.e.

$$U = \tfrac{1}{2} m\omega^2 r^2 + a\mathbf{l}\cdot\mathbf{s}. \tag{3}$$

Further the sign of the parameter a was chosen such that for a nucleon with orbital angular momentum l the state with total angular momentum $j = l + 1/2$ is lower in energy than the one with $j = l - 1/2$. The resulting single nucleon level scheme together with the appropriate quantum numbers is schematically shown in figure 1. If one also ignores the residual interaction term H_1, then one has a simple single-particle model for the nucleus. In this case the figure clearly indicates where the closed shells can occur. An important success of this scheme was the explanation of the "magic" numbers 2, 8, 20, 28, 50, 82, 126 for N and Z. We can, in terms of these numbers, understand why nuclei such as ^{4}He, ^{16}O, ^{40}Ca, ^{208}Pb etc are extra stable. The most important achievement of this extreme single particle model was the correct prediction of the ground state spins and several isomeric states of almost all nuclei which have spherical shape. For this purpose, it is necessary to assume that the nucleons tend to pairwise couple their spins to zero. Therefore, all even-even nuclei have zero spin in the ground state whereas for odd-A nuclei it is given by that of the last unpaired nucleon.

Following the success of this model it seemed natural to extend the model to the

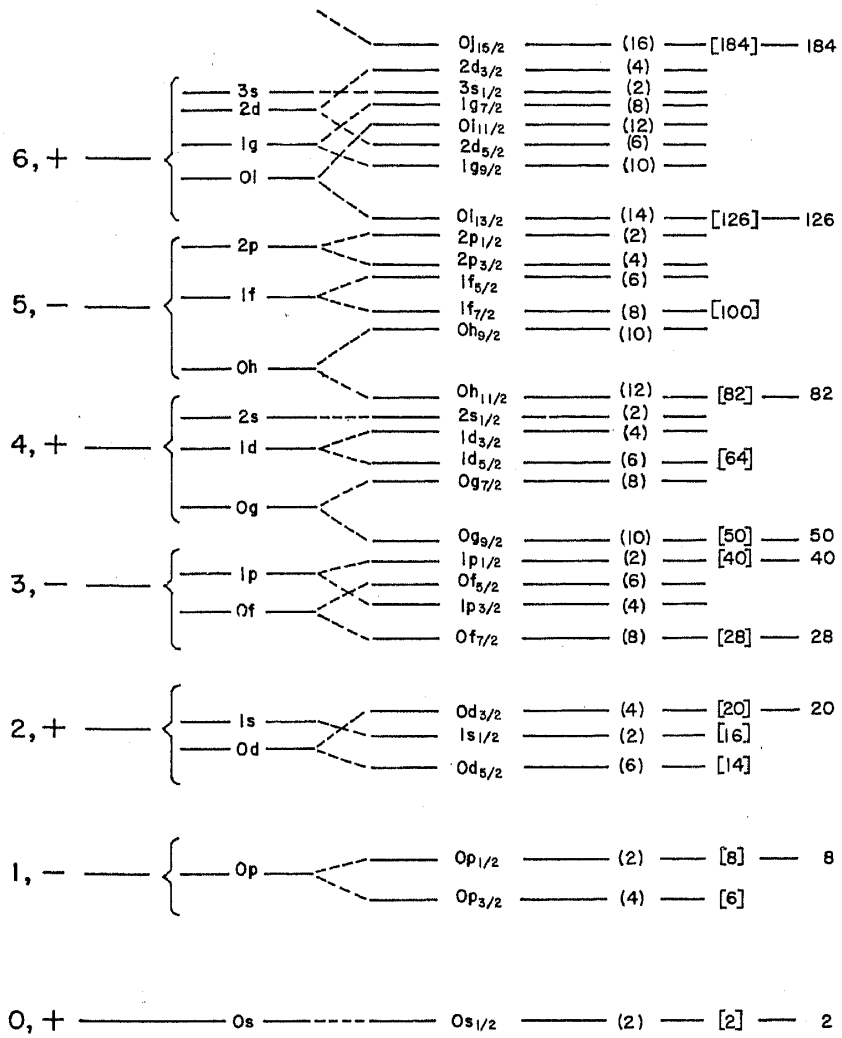

Figure 1. Single-particle level scheme for nuclear shell model (Following Mayer and Jensen 1955 and Pal 1982).

study of the excited states of nuclei. The experimental information at that time was meagre and hence it was adequate to use the simplest extensions of the extreme single particle model. As we shall see this involves extensive use of geometry and symmetry in the problem. It is obvious that to evaluate the energies of excited states the interaction term H_1 in the Hamiltonian must be included.

One of the simplest example of the study of excited levels is in oxygen isotopes (Talmi *et al* 1962). Consider the nuclei ^{18}O and ^{19}O, which respectively have 2 and 3 (valence) neutrons outside of the doubly magic nucleus ^{16}O (see figure 1). Further it is assumed that in these oxygen isotopes, the low-lying excited states are described by configurations in which the double magic ^{16}O core remains inert, and the valence neutrons are confined to the $1d_{5/2}$ orbit. Thus, the configuration for ^{18}O is $(1d_{5/2})^2_J$ $J = 0, 2, 4$ and that for ^{19}O is $(1d_{5/2})^3_J$ $J = 3/2, 5/2, 9/2$. The J-values are the only ones consistent with the Pauli principle. Using the experimentally observed energies, of the $J = 0, 2, 4$ states in ^{18}O, one determines the energies of the ^{19}O states by using

the relation between the energies of n particles in a j-shell with those of $(n-1)$ particles (Talmi *et al* 1962).

$$\langle j^n \alpha J M | H | j^n \alpha' J M \rangle = \frac{n}{n-2} \sum_{\alpha_1 \alpha_1' J_1} (j^{n-1}(\alpha_1 J_1); J | \} j^n \alpha J) \times (j^{n-1}(\alpha_1' J_1); J | \} j^n \alpha J) \langle j^{n-1} \alpha_1 J_1 | H | j^{n-1} \alpha_1 J_1 \rangle. \quad (4)$$

In (4) the left hand side is the energy of the n-nucleon state with angular momentum J. On the right hand side we have the coefficients of fractional parentage which contain the geometry of the problem—i.e. the manner in which the n particle states are built from $(n-1)$ particle states by adding a single particle. The right hand side also has the $(n-1)$ particle energies. Figure 2 shows the ^{18}O (experimental) and ^{19}O (calculated and experimental) spectra which illustrate the application of (4):

Another beautiful example of these simple elegant ideas is the relation between particle-particle and particle-hole spectra (Pandya 1956). One considers here the energy levels of two nucleons with one in orbit j and another in orbit j' and relate them to the energy levels of a nucleon hole in orbit j and a nucleon in j'. Assuming pure $j-j$ coupling and two-body interaction, Pandya (1956) derived the relation

$$E_J[j^{-1}j'] = -\sum_{J_0} (2J_0+1) W(jj'j'j; JJ_0) E_{J_0}[jj']. \quad (5)$$

This was very successfully tested in the spectra of $^{38}_{17}$Cl $(1d_{3/2}\,1f_{7/2})$ and $^{40}_{19}$K $(1d_{3/2}\,1f_{7/2})$ and the results are shown in figure 3. The discrepancy between the calculated and the observed ^{38}Cl spectra is $\lesssim 25$ keV.

Going further, Pandya and French (1956) carried out a more detailed theoretical

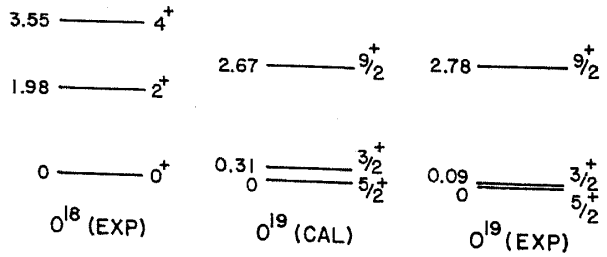

Figure 2. Comparison of calculated and experimental levels of ^{19}O.

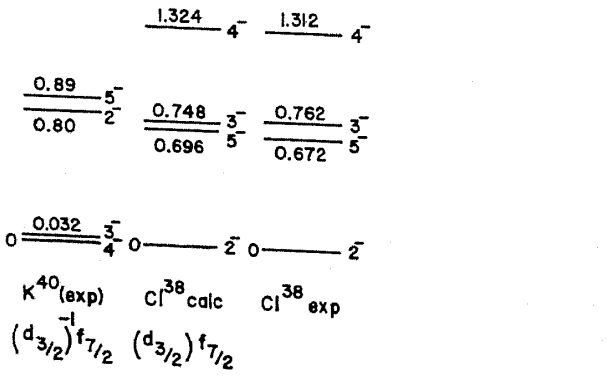

Figure 3. Comparison of calculated and experimental levels of ^{38}Cl.

analysis of the discrepancy, by taking account of contribution to the energies coming from other configurations and argued that the remaining discrepancy may be attributed to 3-body forces. In this case they estimated that 3-body forces contribute between 50 and 250 keV to the energy levels of ^{40}K.

The success of these simple elegant models to reproduce the observed spectra, the development of Brueckner's approach to deduce effective nucleon-nucleon interaction in a nucleus from the bare nucleon-nucleon interaction and the increasing availability of spectroscopic data and high speed computers led to the modern day shell-model activity. This is discussed in §3.

3. Shell model—current status

The basic features of the shell-model today are

(i) Assumption of an inert core for nucleons—i.e. the configuration for a given nucleus (with Z protons, N neutrons, $N+Z=A$) is partitioned into an inert core part (containing Z_c protons, N_c neutrons, $Z_c+N_c=A_c$) and an active valence part (containing $Z-Z_c$ and $N-N_c$ protons and neutrons respectively). For practical reasons the number of valence nucleons must be small, as the numerical computations increase dramatically in magnitude with this number.
(ii) Valence nucleons move in a finite number (often those in a major shell) of j-orbits.
(iii) The Hamiltonian of the valence nucleons is given by

$$H = E_0 + \sum_i \varepsilon_i a_i^+ a_j + \tfrac{1}{2}\sum_{ijkl} \langle ij|v|kl\rangle a_i^+ a_j^+ a_l a_k, \tag{6}$$

where E_0 is the energy of the inert core, ε_i's are the single particle energies of the valence orbits and $\langle ij|v|kl\rangle$ are the matrix elements of the 2-body residual interaction amongst the valence particles. ε_i's effectively take account of interaction between a valence particle and those in the inert core; in practice these are taken from the experimentally observed energy levels of (closed shell) + 1 valence nucleon. v is taken from theoretical calculations or phenomenological models.
(iv) With these assumptions the Schrödinger equation is exactly set up in the model space and solved. Given a suitable basis (say harmonic oscillator states) one obtains eigenvalues and eigenvectors by diagonalizing the H-matrix. The eigenvectors in turn are used to obtain matrix elements of other physically interesting operators such as electric and magnetic moments, EM transition probabilities, β-decay matrix elements, one- and two-nucleon transfer probabilities, etc.
(v) Finally, the shell-model calculations are confronted with *all* the available data. A commonly used procedure is to parametrize the effective interactions (and even single particle energies of valence orbits) and other such operators (M1, GT, E2 etc.) and then obtain the values of these parameters which give the best numerical fit to the observed set of data points.

Such a comparison provides the most detailed and the least model-dependent test of the theory. The objective of most of the shell model calculations todate has been two-fold:

(i) To understand systematically and comprehensively, as many properties of as many nuclei as possible, first with a small sample, and then by expanding it to larger regions

till the model breaks down. Such detailed comparison between calculated and observed data covering large samples will not only establish the validity of the model, but will also eventually expose its limitations, and through examples where the model fails, will show need for including new physics. For example, discrepancy of shell model calculations with observations in highly neutron-rich isotopes of Na or Mg shows the possibility that in such cases $N = 20$ may not be a good magic number, and the whole underlying picture of spherical shell model orbits may have become invalid. Other calculations of Gamov–Teller decay rates etc show the need for including larger configuration spaces, mesonic current effects, etc.

(ii) To deduce the properties of the model interactions (and also other operators) in the assumed configuration space. The important questions here are: is the effective interaction unique? how "universal" is it? can it help to distinguish between different bare NN interactions proposed? (through, off-the-energy-shell effects, perhaps!), is there any signature of density-dependence or many-body terms in such interactions? and a host of other such theoretical points.

It should be stressed that such a programme has been exhaustively pursued only for nuclei in the $2s-1d$ shell—i.e. for $8 < Z, N < 20$. Computer programs to construct and diagonalize Hamiltonian matrices have been in existence for almost 20 years now. The most durable of these have been the Oak–Ridge–Rochester (French *et al* 1969) code (an improved modern version is OXBASH) and the Glasgow code (Whitehead *et al* 1977). The former code is in the angular momentum coupled (J) scheme whereas the latter is in the uncoupled (M) scheme. Some of the earlier work in $2s-1d$ shell is reviewed by Halbert *et al* (1971).

During the past 15 years or so there has been a concerted effort by Wildenthal and his collaborators to obtain interactions which will reproduce the experimental results throughout the $2s-1d$ shell nuclei. In their early work they had different interactions for the lower ($18 \leqslant A \leqslant 22$) and the upper ($32 \leqslant A \leqslant 38$) parts of the $2s-1d$ shell (Preedom *et al* 1972, Chung *et al* 1979). More recently Wildenthal (1984) took the 3 s.p. energies and the 63 (JT-coupled) two-body matrix elements in the $2s-1d$ shell as free parameters, and varied them to give a best fit to the binding energies and excitation energies of about 440 levels throughout the $2s-1d$ shell. The r.m.s. deviation was found to be about 150 keV. It ought to be mentioned that the two-body matrix elements were taken to be A-dependent; more precisely they took

$$(V)_A = (V)_{A=18}(18/A)^{0.3}. \tag{7}$$

In addition, the two neutron separation energies were calculated for this interaction with the same kind of deviation (~ 150 keV) in most cases. This is shown in figure 4. The interaction has also been used to study magnetic moments, M_1 transition, and beta decay strengths. A comparison of the experimental and theoretical beta decay strengths (summed over the final states) is shown in figure 5. Again the agreement is quite impressive (see Brown 1987 for highlights of the calculations using the above mentioned interaction).

Recently Fiase *et al* (1988) tried to generate a simple A-dependent effective interaction starting from a more fundamental approach. They use the Reid soft-core potential together with a set of correlation functions to simulate the effect of the nuclear medium to deduce an effective Hamiltonian for the $2s-1d$ shell nuclei. They write

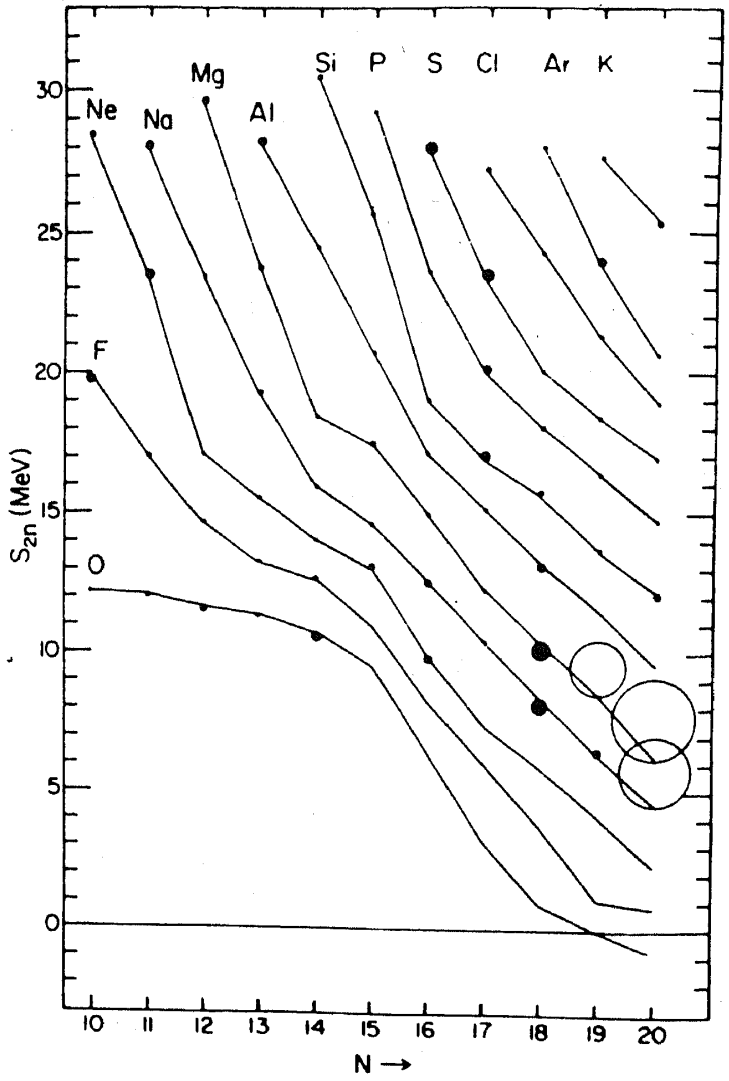

Figure 4. Two neutron separation energies for nuclei in $2s-1d$ shell (from Brown 1987).

$$H_{\text{eff}} = \sum_{i<j} f_{ij}(H)_{\text{bare}} f_{ij}, \tag{8}$$

where f_{ij} are the two-body correlation operators and assumed to have the form (Fiase *et al* 1988)

$$f_{ij} = f(r_{ij}) \sum_{\lambda} (1 + \alpha_{\lambda}(A) S_{ij}), \tag{9}$$

where λ denotes a reaction channel and S_{ij} is the usual tensor operator. $f(r_{ij})$ takes account of short range correlations with the form

$$f(r_{ij}) = 1 - \exp[-\beta(r_{ij} - r_c)^2] \tag{10}$$

and $r_c = 0{\cdot}25\,\text{fm}$; $\beta = 25\,(\text{fm})^2$.

The tensor correlations are assumed to exist in the $(3S_1 - 3D_1)$ channel only and hence the parameter $\alpha_{\lambda}(A) = 0$ unless $\lambda = 3S_1 - 3D_1$. This parameter $\alpha(A)$ is determined by fitting to nuclear properties in different nuclei to obtain its A dependence.

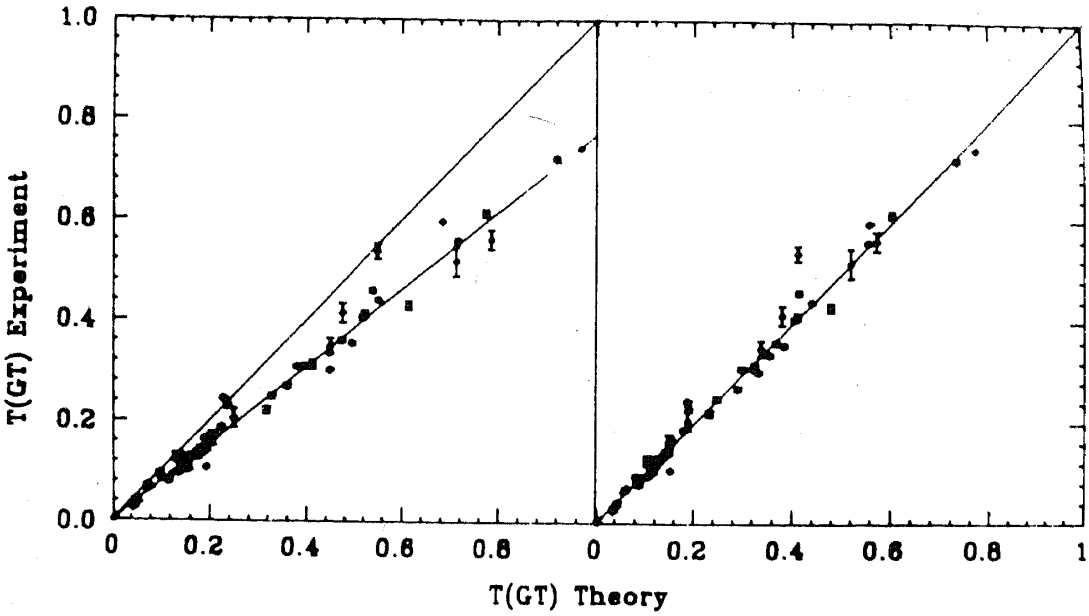

Figure 5. Theoretical vs experimental T(GT) matrix elements (from Brown 1987).

It was found to be a monotonically decreasing function of A with $\alpha(A=4)=0{\cdot}1$, $\alpha(A=16)=0{\cdot}08$ and asymptotically $\alpha(A\to\infty)=0{\cdot}06$.

A comparison of these matrix elements was made with those of Preedom and Wildenthal (1972), Chung *et al* (1979) and Wildenthal (1984). It is found that for $18\leqslant A\leqslant 22$ the effective interaction of Fiase *et al* (1988) is in excellent agreement with that of Preedom and Wildenthal and for $32\leqslant A\leqslant 38$, the effective interaction is in agreement with that of Chung *et al* (1979). The agreement with the matrix element of Wildenthal (1984) is not as good. In addition, these authors (Fiase *et al* 1988) find that only the diagonal matrix elements have the A-dependence whereas the off-diagonal ones do not. The A-dependence of the diagonal matrix element has the scaling factor $(18/A)^{0{\cdot}3}$ found by Wildenthal (1984).

It seems therefore that the shell-model programme in the $2s-1d$ shell has to a large extent been successfully implemented. The p-shell nuclei are much simpler, and have succumbed to shell model much earlier. Even the nuclei spanning the p- and the sd-shell have been successfully described (Millener and Kurath 1975).

4. Future of shell-model

From the achievements of the shell-model (Brown 1986; Fiase *et al* 1988) in the $2s-1d$ shell, it seems natural to extend the programme to heavier nuclei. The next logical region to attack is the fp shell, with $40<A<56$. Brown, Wildenthal and collaborators have undertaken an extensive programme to extend their "universal" sd shell interaction to this region. There is certainly a lot of experimental information which can be correlated and perhaps reasonable confidence about the manner in which the effective interaction can be obtained in view of the recent work of Fiase *et al* (1988). However, in order to implement this traditional shell-model approach in its completeness, a substantial increase in computing power is required. With this requirement in mind the Glasgow group (Mackenzie *et al* 1988) has recently advocated

the use of parallel processing and have designed and constructed a dedicated multiprocessor for shell-model calculations. This would be able to handle matrices of dimensionally 10^6–10^7 in *m*-scheme.

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