PRESENT STATUS OF SHELL MODEL TECHNIQUES*

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The technical problems appearing in Shell Model calculations are discussed. The solutions developped in the codes ANTOINE (m-scheme) and NATHAN (coupled scheme) are explained with a special focus on the treatment of giant matrices. New possiblities, limitations and possible improvements are presented.

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1. Introduction

The Shell Model (SM) has always been considered as a fundamental tool for the study of the nuclear structure. The main reason is that it allows a simultaneous description of all the spectroscopic properties of the low-lying states; with the same valence space and the same effective interaction it can describe the backbending of ^{48}Cr [1] and its half-life [2], the spherical structure of the ground state of ^{56}Ni and its excited deformed band [3].

Two main problems appear in a Shell Model description of the nuclear structure. The first one is related to its very foundations, *i.e.* to the possibility of obtaining a regularized effective interaction in a given valence space, from the bare nucleon-nucleon force. Since the pionnering work of Bruekner [4] this has been a basic theoretical problem and there are still many new developements in this field [5]. In its present state, effective interactions cannot be used in SM calculations without some phenomenological corrections [6].

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The second problem is technical: with the increase of the size of the valence or (and) the increase of the number of particles (holes) the dimensions of the matrices explode.

This explains why SM calculations have been only extensively done :

- For light nuclei, p shell [7] and $s-d$ shell [8].
- For heavy nuclei with only few particles (holes) outside an inert core [9] or for semi-magic nuclei [10, 11].

Progress in the technology of computers can help in extending the range of nuclei amenable to a SM description, however, improvements in the quality of the SM codes will play a prepodominant role. Another avenue is provided by the application of stochastic approaches to this problems, that we shall not discuss here [12, 13]. We shall deal in this article with the recent developments leading to new codes (ANTOINE, NATHAN) that make it possible for example the study of fp shell nuclei [2, 14] reaching m-scheme equivalent dimensions of **one billion**. The article is divided in 4 chapters :

1. The diagonalization method (Lanczos).
2. The choice of the basis and the calculation of the matrix elements (m.e.).
3. The treatment of *giant* matrices.
4. The present possibilities and limitations.

2. The diagonalization (the Lanczos method)

Standard diagonalization methods whose CPU time increases like N^3, N being the dimension of the matrix, cannot be used if one is aiming to large scale SM calculations. Since, in general, only a few eigenvalues and eigenvectors are needed, the LANCZOS algorithm appears as the most suitable and it is in fact the standard method for this kind of problems.

In this method we build an orthogonal basis in which the Hamiltonian H matrix is tridiagonal. We start with a normalized vector (pivot state) Φ_1 and apply the H operator on this vector. Then we get a parallel and an orthogonal components to the initial vector Φ_1:

$$H|\Phi_1\rangle = E_{11}|\Phi_1\rangle + E_{12}|\Phi_2\rangle$$

with $E_{11} = \langle\Phi_1|H|\Phi_1\rangle$ and $E_{12}|\Phi_2\rangle = H|\Phi_1\rangle - E_{11}|\Phi_1\rangle$.

Acting again with H on Φ_2, we generate a third vector Φ_3 orthogonal to the first two.

$$H|\Phi_2\rangle = E_{21}|\Phi_1\rangle + E_{22}|\Phi_2\rangle + E_{23}|\Phi_3\rangle$$

$E_{21} = E_{12}$ since in our basis H matrix is real-symmetric.

Continuing this process, at iteration n, we obtain the diagonal energy of the vector $|\Phi_n\rangle$, a new vector $|\Phi_{n+1}\rangle$ and the non diagonal energy $E_{n\ n+1}$.

$$\begin{aligned} H|\Phi_n\rangle &= E_{n\ n-1}|\Phi_{n-1}\rangle + E_{nn}|\Phi_n\rangle + E_{n\ n+1}|\Phi_{n+1}\rangle\,, \\ E_{n\ n-1} &= E_{n-1\ n}, \quad E_{nn} = \langle\Phi_n|H|\Phi_n\rangle\,, \\ \text{and } E_{n\ n+1}|\Phi_{n+1}\rangle &= H|\Phi_n\rangle - E_{nn}|\Phi_n\rangle - E_{n\ n-1}|\Phi_{n-1}\rangle\,. \end{aligned}$$

Due to the hermiticity of H, the construction of the Lanczos matrix ensures that all the elements E_{ij} with $|i-j| > 1$ are zero.

This iterative process will continue until all the eigenvalues that we need are converged. For this reason the choice of the pivot state is crucial. Here are some ideas to accelerate the convergence:

- To restore the good quantum numbers in the pivot state. For example, in m-scheme, we project the pivot state on J^2 and T^2 (this projection is achieved in doing a Lanczos calculation with the J^2 and T^2 operators).
- Especially when we need only one converged state, it is interesting to use as pivot state the solution obtained in a truncated space. For example if we want to calculate the Yrast band of ^{50}Cr in the full pf space (dimension in m-scheme 14,625,540) we will first do the calculation in a space in which only 4 particles are outside the $f_{7/2}$ shell (dimension 1,856,720). The overlap between the two 0^+ states being 0.985, we will obtain the converged result with a much smaller number of iterations.

An important point to notice is that all the Lanczos vectors must be kept during the calculation. There are two reasons for this; firstly, we need them to calculate the eigenvectors and secondly because of numerical reasons. Mathematically the Lanczos vectors should be orthogonal, however numerically this is not strictly so. Hence, small numerical precision errors can, after some iterations, produce catastrophes (*e.g.* the lowest states may reappear many times). To avoid that it is necessary to reorthogonalize each new Lanczos vector to all the precedent. The necessity of keeping all these vectors can be, for huge matrices, a real problem. As we will see, in the m-scheme code, it is actually the most important element limiting its possibilities.

3. The choice of the basis

For a given valence space, the choice of of the basis is only a problem of convenience. As it will be discussed later, depending on what we want to describe (ground state, yrast band, strength function ...) one or another basis will be more appropriate. There are basically two possibilities:

- the m-sheme,
- the coupled scheme (J or JT).

In m-scheme, the states of the basis are Slater Determinants (SD) of A particles distributed in k individual orbits $|nljm\tau\rangle$.

$$\Phi_{a_1 \ldots a_A}(1, ..., A) = \det \{\phi_{a_k}(r(k)\} = \prod_k a^+_{a_k}|0\rangle \, .$$

The fundamental advantage of this representation is the simplicity of the calculation of the many particle m.e. of H, because they reduce to the two-body m.e. of H in m-scheme with a phase. It means that, independently of the size of the matrix, the number of possible values of non-zero m.e. is relatively limited.

Based on these ideas, the **Glasgow** group wrote, some 20 years ago, a very clever (because very simple) SM code [15]. In it, each SD was represented in the computer by an integer word and each bit of the word associated to a given individual state $|nljm\tau\rangle$. Each bit has the value 1 or 0 depending on whether the state is occupied or empty. A two-body operator $a^\dagger_i a^\dagger_j a_k a_l$ will search the words having the bits i, j, k, l in the configuration 0011 and change it to 1100. This generates new words which have to be located in the list of all the words by the bi-section method.

However the counterpart of the simplicity of the m-scheme is that only J_z and T_z are good quantum numbers, therefore all the possible (J, T) states are in the basis and as a consequence the dimensions of the matrices are maximal, being proportional to the product of the two combinatorial numbers made with the total degeneracy of the proton (neutron) valence spaces and the numbers of active protons (neutrons).

The J or JT coupled basis, splits the full m-scheme matrix in boxes whose dimensions are much smaller. This is especially spectacular for the $J = 0$ states (see Table I).

In the late 60's, the Rochester group developped the formalism needed for an efficient work in a (J, T) coupled basis and applied it in the **Oak-Ridge Rochester Multi-Shell** code [16]. The procedure is now the following:

Firstly the states of n particles in a given j shell are defined: $|\gamma_i\rangle = |(j_i)^{n_i} v_i J_i x_i\rangle$ (v_i is the seniority).

TABLE I

Dimensions in pf shell

A	4	8	12	16	20
$M_z = T_z = 0$	4000	$2*10^6$	$1.10*10^8$	$1.09*10^9$	$2.29*10^9$
$J = T_z = 0$	156	41355	$1.78*10^6$	$1.54*10^7$	$3.13*10^7$
$J = T = 0$	66	9741	$3.32*10^5$	$2.58*10^6$	$5.05*10^6$

Then the k-shell states are obtained by successive angular momentum couplings of the one-shell basic states. $\left[\left[\left[|\gamma_1\rangle|\gamma_2\rangle\right]^{\Gamma_2}|\gamma_3\rangle\right]^{\Gamma_3}\ldots|\gamma_k\rangle\right]^{\Gamma_k}$

Compared to the simplicity of the m-scheme, the calculation of the non-zero multiparticle matrix elements is much more complicated. These m.e. involve products of cfp's and $9j$ coefficients.

However, in the case of only J (without T) coupling, a strong simplification in the calculation of these m.e. can be achieved using the quasi-spin [17] formalism.

The one-shell states are now written as $|S_i S_{zi} J_i x_i\rangle$ instead of $|n_i v_i J_i x_i\rangle$. S_i and S_{zi} are defined by:

$$S_i = \frac{\Omega_i - v_i}{2}, \quad S_{zi} = \frac{\Omega_i - n_i}{2},$$

where $2\Omega_i = 2j_i + 1$ is the degeneracy of the shell j_i.

The quasi-spin operators close an SU(2) algebra. The application of the Wigner–Eckart theorem makes possible to use doubly reduced (in spin and quasi-spin) cfp's.

Defining $S \equiv (S_1, S_2, ..., S_k)$ (idem for S_z, J, x, Γ) the expectation value of an operator O reads : $\langle S S_z J x \Gamma || O || S' S'_z J' x' \Gamma' \rangle = \langle S J x \Gamma || | O | | | S' J' x' \Gamma' \rangle \times CG(S_z, S'_z)$

For a given S, we have p states $Jx\Gamma$ and q states. To get the matrix $p \cdot q \times p' \cdot q'$ we calculate **separately** the matrices :

- $p \times p'$ doubly-reduced m.e. ,
- $q \times q'$ product of Clebsh–Gordan coefficients.

This factorization reduces by a huge factor the computing time (for more details see Ref. [18]).

4. The treatment of giant matrices

When it is said that a matrix is giant, it is not a qualitative but a quantitative definition. It means that there are so many non-zero elements in the matrix that they cannot all be stored on the disks of the computer. This is the fundamental limitation of the old shell model codes. To give an order of magnitude, the 0^+'s of ^{112}Sn in the $g_{7/2}, d_{5/2}, d_3/2, s_{1/2}, h_{11/2}$ space have dimension 136,940 and 346,627,207 non-zero m.e. in the coupled basis.

This means that for giant matrices it is necessary to recalculate the m.e. in the diagonalization itself. Modern shell model codes must tackle this problem and the quality of the code will be directly related at its performance in the calculation of non-zero terms during the Lanczos procedure.

The first breakthrough in this direction was achieved by the Glasgow group [15]. Their method to generate non-zero m.e. (see precedent chapter) is so simple that it was just included in the Lanczos algorithm.

A. The *m*-scheme code ANTOINE

This SM code was based in Glasgow's ideas. It takes advantage of an important progress which appeared in the technology of computers some years after the writing of the Glasgow code, the virtual memory which allows to store many precalculated results.

The improvements over the Glasgow code are the following :

In the valence space there are protons and neutrons. Even for large dimensions in the total space, the dimensions in the proton and neutron spaces separately are small. For example, the 1,963,461 SD with $M = 0$ in ^{48}Cr are generated with only the 4,865 SD (all possible M values) in ^{44}Ca.

A basis state is now written as the product of the SD of protons and neutrons.

$|I\rangle = |i, \alpha\rangle$, where we use

I, J capital letters for states in the total space ,

$i, j \ldots$ small case latin letters for proton states ,

$\alpha, \beta \ldots$ small case greak letters for neutron states.

The i and α SD can be classified by their J_z values M_p and M_n. The total M being fixed, SD's for p and n will be associated only if $M_p + M_n = M$. An example is given in Fig. 1.

If we make a loop on i, and then on α, we see in our example that since we have 4 states α in the first "block" (M_p, M_n) the SD $i = 1$ generates states $I = 1, 2, 3, 4$ $i = 2$ generates $I = 5, 6, 7, 8$ and so on.

When we arrive to the second "block" $(M_p + 1, M_n - 1)$, $6 * 4 = 24I$ states have been built. Next we have here 3 states α, it means that $i = 7$ generates $I = 25, 26, 27$. It is clear that for each i state the allowed α states go **without discontinuity** between a minimum and a maximum values,

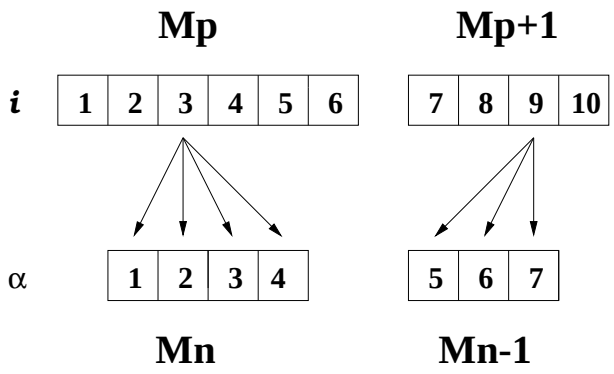

Fig. 1. Schematic representation of the basis.

therefore it is possible to construct **numerically** an array $R(i)$ so that :

$$I = R(i) + \alpha\,.$$

In our example we have $1 = R(1) + 1,\ 5 = R(2) + 1,\ 25 = R(7) + 5,\ ...$ So having i, α and $R(i)$ we can get immediately I. Afterwards, the program proceeds as follows :

For the pp and nn m.e. all the $(R(i),\ R(j),\ W)$ and $(\alpha,\ \beta,\ W)$ where $\langle i|H|j\rangle = W$ and $\langle\alpha|H|\beta\rangle = W$, are precalculated and stored. Therefore, in the Lanczos procedure a simple loop on α and i will generate all the pp and nn m.e. (I, J, W). For instance, in the ^{48}Cr case, 102,886 (i, j, W) terms generate 46,484,396 (I, J, W).

For the pn matrix elements the situation is only a bit more complicated. Lets assume the ths SD i and j are connected by the one-body operator $a_q^\dagger a_r$ (labeled by p), with $q = nljm$ and $r = n'l'j'm'$ and $m' - m = \Delta m$. We precalculate all the $(R(i), R(j), p)$ and (α, β, μ). Conservation of the total M implies that the proton operators with Δm must be associated at the neutron operators with $-\Delta m$. Thus we could draw the equivalent to figure 1 for the p and n one-body operators. In the same way as we did before for $I = R(i) + \alpha$, we can now define $K = Q(p) + \mu$. $V(K)$ would be the two-body proton-neutron m.e. that connect the states (i, α) and (j, β).

Once $(R(i),\ R(j),\ Q(p))$ and $(\alpha,\ \beta,\ \mu)$ stored, the non-zero elements of the matrix in the full space are generated with 3 integer additions:

$$\begin{aligned} I &= R(i) + \alpha\,, \\ J &= R(j) + \beta\,, \\ K &= Q(p) + \mu\,, \\ H_{I,J} &= H_{J,I} = V(K)\,. \end{aligned}$$

B. The coupled code NATHAN

We can apply the same basic idea ($p-n$ factorization) to the J-coupled formalism. Now instead of M_p and M_n we have J_p and J_n. The difference is that for a given J_p we have many J_n, but we will maintain the continuity between the first state with $J_{\min}$ and the last with $J_{\max}$. As a consequence the fundamental relation $I = R(i) + \alpha$ still holds.

The generation of the $pp(nn)$ m.e. is exactly as for the m-scheme. The pn operators are now $(a^\dagger_{j_1} a_{j_2})^\lambda$ and we have a strict analogy between Δm in m-scheme and λ in the coupled scheme. It means that we can yet write $K = R(p) + \mu$.

However, the proton-neutron m.e. are not so simple. They now read:

$$H_{I,J} = H_{J,I} = h_{i,j} * h_{\alpha,\beta} * W(K)\,,$$

where $h_{i,j}$ and $h_{\alpha,\beta}$ are the mean values of the one-body operators (a kind of generalized cfp coefficients), $W(K)$ is the product of the two-body m.e. with the $9j$ coefficient for the coupling of the proton and neutron wave-functions. Therfore, the generation of the proton-neutron m.e. demands three integer additions as in the m-scheme code, plus two floating point multiplications.

5. Possiblities, limitations, perspective

The largest calculation done with the code ANTOINE is the yrast band of ^{52}Fe (including the isomeric state $J = 12^+$) [19]. Choosing $J_z = 0$ and taking into account for $M_p \neq 0$ the time reversal symmetry we have to deal with a dimension 62,786,462 . The equivalent of 17 millions of integer words (precalculated and stored) allow the generation of the $75 * 10^9$ non-zero terms in the Lanczos procedure. In the present version of the code two Lanczos vectors must be simultanously resident in the memory and the limitation is clearly there and not in the calculation itself.

In the coupled scheme we have the opposite situation. The dimensions are never a problem so that we have been able to calculate the ground state of ^{56}Ni (dimension 15,443,684 but 10^9 in m-scheme) [20]. Here the limitation comes from the huge number of non-zero terms related at the multiplicity in λ. To come back at the example of ^{52}Fe, the 0^+ state has dimension 1,777,116 and $180 * 10^9$ non-zero terms, the 6^+ state has dimension 11,909,614 and $6.5 * 10^{12}$ non-zero. We then see that the two codes are complementary, the coupled one will be preferable for small spins or when a lot of Lanczos iterations are needed as for the calculation of strength function [21]. It has also the possibility to incorporate seniority truncations which is interesting for heavier spherical nuclei.

A common weakness of the two codes appears when the spaces generated by protons and neutrons are too asymmetric. For semi-magic nuclei, the codes calculate and store all the non-zero terms of the matrix. Sn or Pb isotopes are not our favourite nuclei.

Some improvements can be envisaged:

- In some cases Davidson method can be better than Lanczos, accelerating the convergence and avoiding the storage of numerous huge vectors [22].
- The Lanczos algorithm is relatively easy to parallelize. The generation of the $H_{I,J}$ can be shared between different processors.
- Reasonable approximations on H can simplify strongly the calculation.

  In the m-scheme a separable (even a sum of) proton-neutron interaction can simplify strongly the calculation, by **succesive** application of the p and n operators. The J^2 operator is calculated with this method.

  For the coupled code some λ can certainly be forgotten. As an example we consider the ground state of ^{82}Kr in the full . $p_{3/2}f_{5/2}p_{1/2}g_{9/2}$ space (dimension of the matrix 783,879 with $27.5 * 10^9$ non-zero).

TABLE II

Number of terms (percentage) and energy contribution

λ	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+
non-zero (%)	0.7	3.3	3.6	3.5	1.4	1.2	0.7	1.0	0.5
energy (kev)	-3.	-8040.	-1.	-350.	11.	-8.	0.4	1.	0.4
λ	2^-	3^-	4^-	5^-	6^-	7^-			
non-zero (%)	2.7	12.1	23.9	25.2	15.2	5.1			
energy (kev)	1.	-468.	4.	-322.	6.	-153.			

We give in Table II the number of terms (percentage) and the contribution to the energy of each λ coupling of the proton-neutron interaction.

- For very asymmetric p and n space, other factorizations (shells) could be more favorable and the possiblility of a (J,T) coupled code along these lines is under consideration.

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