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Truncation method for shell model calculations

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A method of truncating the large shell model basis is outlined. It relies on the order given by the unperturbed energies of the basis states and on the constancy of their spreading widths. Both quantities can be calculated by a simple averaging procedure. The method is tested in the *sd* shell where the JT dimensions are of the order of a few thousand. It proves to be very effective in the middle of the *fp* shell where JT dimensions of the order of a few times 10^6 are truncated to a few times 10^3.

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Shell model calculations of the ground state and low-lying excited states are of interest for our understanding of nuclear dynamics and the (effective) nuclear forces. They are also of great interest for the prediction and analysis of various processes (Gamow-Teller rates, parity nonconservation matrix elements, electromagnetic transition probabilities, isospin breaking matrix elements, spectroscopic factors, etc.) important for nuclear astrophysics and tests of the fundamental interactions in nuclei. Unfortunately, even for light nuclei, the large model-space dimensions present a challenge for the traditional diagonalization methods (see, e.g., Ref. [1]). During the last few years other approaches to this problem have been vigorously investigated [2,3].

In this work we outline a quantitative method of truncating the nuclear shell model spaces to manageable sizes. To achieve this we show that the basis states, whose unperturbed energies (the diagonal matrix element of the Hamiltonian) are far away from the lowest one, give relatively small contributions to the structure of the ground states and low-lying excited states. This statement can be quantified due to an interesting property of the squared amplitudes of the basis states (denoted by the index k), $|C_k^\alpha|^2$, as a function of the eigenvalues, E_α. Figure 1 presents two of these distributions for the basis state number 2 (left) and for the basis state number 825 (right). The basis states are ordered by the JT dimension of the partition (distribution of particles in the single particle levels) to which they belong. The largest partitions are those on the left-hand side of the k axis in Fig. 2 (the dimension of partitions is proportional to the length of the horizontal thick lines in this figure) while the smallest partitions are those on the right side of the k axis. Basis state number 2 belongs to the largest partition, which is situated in the middle of the unperturbed spectrum ($\bar{E}_k$ in Fig. 2), while the basis state number 825 belongs to a small partition whose unperturbed energy is closer to the lowest eigenenergy. We note (see left-hand side of Fig. 1) that the contribution of the basis state number 2 to the ground state ($E_1 = -135.9$ MeV) is small. One observes that the distributions of $|C_k^\alpha|^2$ are close to a Gaussian. It is straightforward to show that their mean values (centroids) are given by the diagonal matrix elements of the Hamiltonian

$$\bar{E}_k \equiv \sum_\alpha |C_k^\alpha|^2 E_\alpha = H_{k,k} \tag{1}$$

and the widths are given by

$$\sigma_k \equiv \sqrt{\sum_\alpha |C_k^\alpha|^2 E_\alpha^2 - \bar{E}_k^2} = \sqrt{\sum_{k' \neq k} H_{k',k}^2}. \tag{2}$$

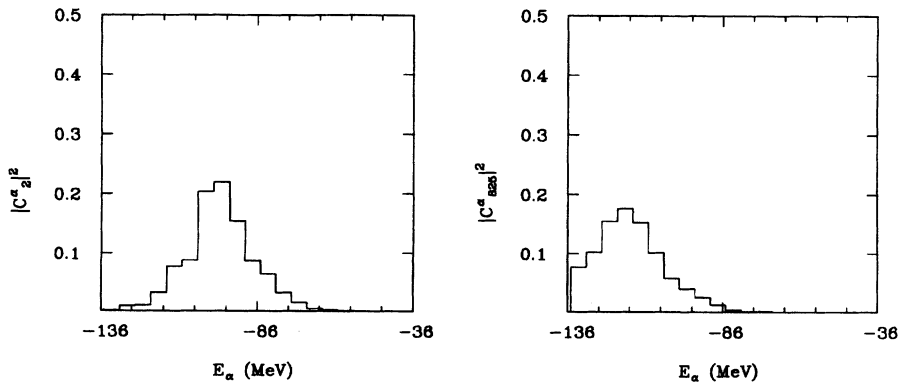

FIG. 1. $|C^\alpha|^2$ vs E_α for basis state number 2 (left) and basis state number 825 (right).

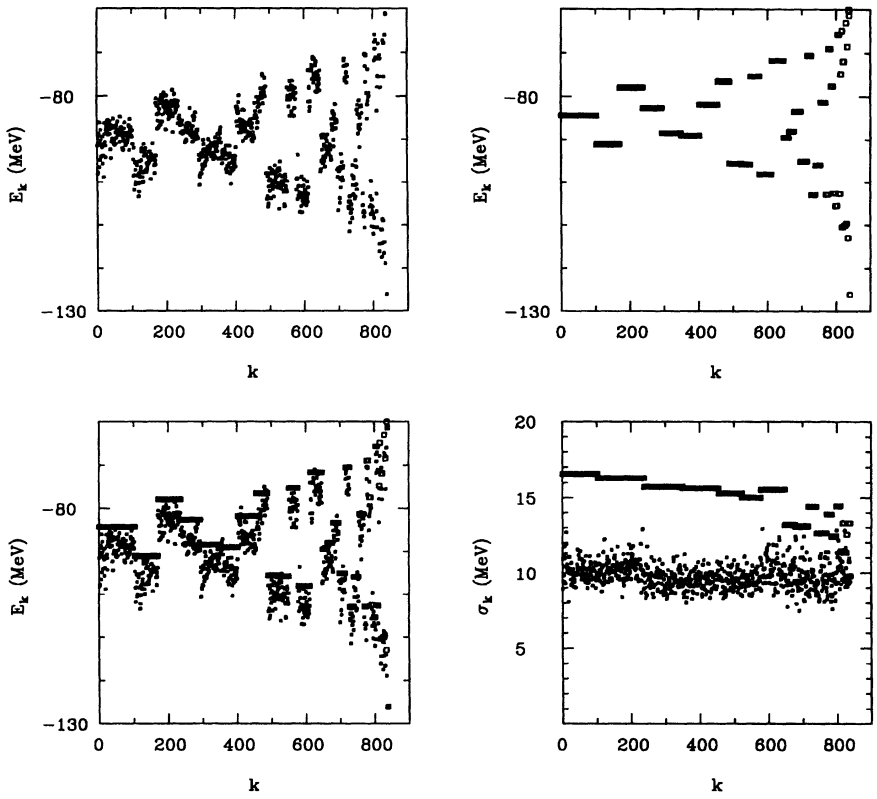

FIG. 2. Energy centroids and σ widths of the basis states coefficients distribution [see Eqs. (1) and (2)].

The small squares in Fig. 2 represent these quantities for the case of 12 particles in the *sd* shell with $J^{\pi}T=0^{+}0$. The Wildenthal interaction [1] has been used for this plot. We have also used different interactions and have carried out calculations in the *fp* shell, but the results are qualitatively the same. To obtain the points, no diagonalization is necessary but only a knowledge of the Hamiltonian matrix as given in Eqs. (1) and (2). Due to the empirical fact that σ is nearly constant for all basis states we can, for example, consider only those basis states whose centroids are lower than $H_{\text{cutoff}}=(\bar{E}_k)_{\min}+3\bar{\sigma}$, where $\bar{\sigma}$ is an average value for σ_k.

One would like also to avoid the construction of the large Hamiltonian matrix. A useful procedure is to use some average values for the quantities in Eqs. (1) and (2). One simple way to proceed is to use the *m*-scheme average values given by French and Ratcliff [4]. They are presented in Fig. 2 by the big squares. (For clarity, the two upper panels decompose the lower left-hand panel in two components: the left for the exact centroids and the right for the French and Ratcliff averages.) They are constant within every partition. The average values slightly overestimate the exact values due to the fact that they are derived for the *m* scheme, whereas the physical states we work with are projected onto good angular momentum and isospin. However, the *m*-scheme estimate is good enough for our purpose.

Our method consists of retaining only those partitions whose average centroids (calculated with the approximate formulas [4]) are smaller than H_{cutoff}. The method has the advantage that one can include step-by-step new partitions in the order of their centroids. We have tested the method in the *sd* shell where we know the exact results. In Fig. 3 we show the results for the lowest $0^{+}1$ states in the case of 10 particles in the *sd* shell [$\bar{\sigma}=9.7$ MeV, $(\bar{E}_k)_{\min}+3\bar{\sigma}=-66.5$ MeV which corresponds to a dimension of 310 in Fig. 3]. The left part of Fig. 3 shows the eigenvalues of the ground state and first excited state as a function of dimension of the

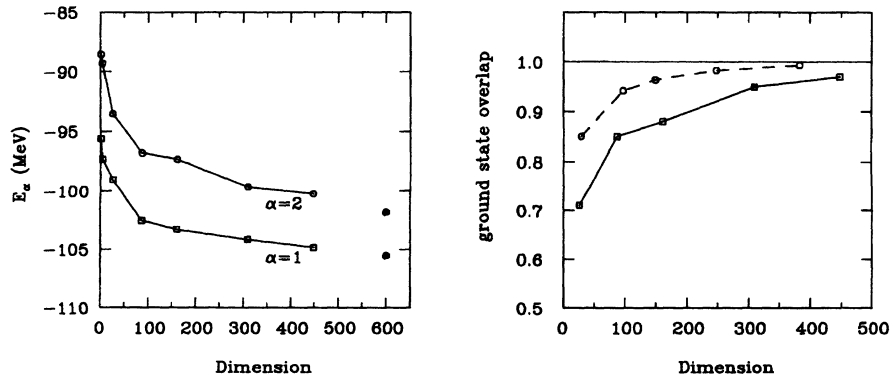

FIG. 3. Energies of the two low-lying states vs the dimension of the truncated space (left); overlaps of the truncated space wave functions with the exact ones (right).

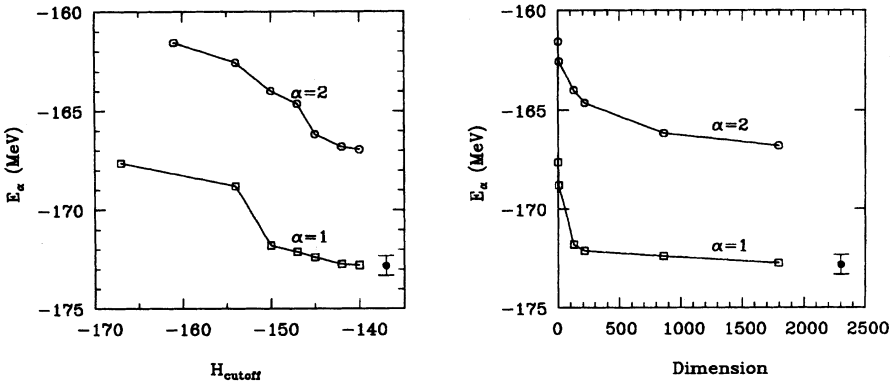

FIG. 4. Energies of the first two low-lying states of ^{54}Fe as a function of truncation diagonal matrix element (left) and vs the dimension of the truncated space (right). The filled circles with the error bars are the result of a recent Monte Carlo calculation [6].

truncated space. The dimension of the full space is 1132. The filled circles (to the right) are the exact values. One can see that with relatively truncated spaces one can approach the exact eigenvalues. To have another measure of the precision of the method, we plot in the right-hand part of Fig. 3 the overlaps of the approximate ground state wave function with the exact ground state wave function (full line). One can see that with less than 30% of the full dimension one can obtain more than 90% overlaps. The dashed line represents the "optimal" truncation in the sense that we retained only those basis states whose exact amplitudes are the highest. One can see that our simple truncation procedure is near to the "optimal" one.

Our investigations in the *sd* shell (maximum JT dimension of the order of a few thousand) show that by using this method one can reduce the dimension of the Hamiltonian matrices by typically a factor of 3. Going to larger model spaces one might expect this factor to be even higher, particularly in cases where simple shell model configurations (e.g., those with the lowest E_k in the left-hand side of Fig. 2) represent a reasonable approximation to the exact ground state wave function. As an example we investigated the 0^+1 low-lying states of ^{54}Fe (14 particles in the fp shell, with the Brown-Richter interaction [5]) using our truncation method. The dimensions of the problem make the traditional calculations unmanageable, even with the next generation of computers: 2229178 JT dimension and 345400274 m-scheme dimension. The results of our truncation method are presented in Fig. 4 [$\tilde{\sigma}=8$ MeV, $(\tilde{E}_k)_{\min}+3\tilde{\sigma}=-143.6$ MeV]. We do not have exact results with which to compare, but we can refer to the result of a recent Monte Carlo calculation [6] indicated by the filled circles with errors bars in Fig. 4. The comparison is encouraging, and our method should allow the calculation of energies to within less than 1 MeV accuracy for the ground states and low-lying excited states for even larger model spaces.

Usually, the shell model spaces are truncated according to some qualitative scheme by retaining only the lowest Hartree-Fock configuration and some simple one-particle–one-hole (1p-1h) or 2p-2h configurations (see, e.g., Ref. [7] for a recent survey of this method in the fp shell). These methods are useful for some particular class of problems; they are a straightforward extension of the Tamm-Dancoff approximation. They do not fully take into account the details of the interaction between the valence particles. Our method is more general; it selects the most important partitions determined by the interaction, and it is suited for a hierarchy of successively better approximations.

A model which has some similarities with our method has been presented in Ref. [8] and slightly refined in Ref. [9]. The crucial differences between our approach and that given in Ref. [9] are the following: (i) We have proposed a general quantitative criteria for selecting the most relevant configurations based on the σ widths given by the off-diagonal matrix elements of the Hamiltonian. The criteria used in Ref. [9] were based on the observation that one can use the lowest 33% of the total configuration as a reasonable approximation for model spaces with JT dimensions of the order 1000–2000. Our findings coincide with those from Ref. [9] for similar dimensions but diverge in some cases for larger dimensions. (ii) The truncation scheme of Ref. [9] was useful only to reduce the diagonalization process; the JT basis states are still necessary. Our truncation scheme is able to select the most relevant partitions before the basis state construction, thus avoiding the calculation of all diagonal matrix elements of the full Hamiltonian (which is the most time consuming part for any shell model calculation).

Our method works well in a full major harmonic oscillator shell ($0\hbar\omega$ calculations), where the spurious center-of-mass motion factors out. The standard method of removing the center-of-mass spurious components of the shell model wave functions, when many $n\hbar\omega$ excitations are included, is to add to the nuclear Hamiltonian, H_N, the center-of-mass Hamiltonian, $H_{\text{c.m.}}$, multiplied by a large constant [10]. In this case the matrix elements of $H_{\text{c.m.}}$, which dominates, are different from that of the nuclear part, and the method described above cannot be directly applied. One way to circumvent this difficulty is to use our method to select the most important partitions by taking into account only the nuclear Hamiltonian, H_N. The part proportional to $H_{\text{c.m.}}$ is included only during the diagonalization in the truncated basis. A calculation in ^{14}N [$(0+2+4)\hbar\omega$], using this scheme reproduces the energy of the 0^+1 yrast state within 400 keV with a JT dimension of the truncated space which is one-fifth of the dimension of the full space (19 498). Work in this

direction is in progress.

We also note that the present method might be used as a criteria for an importance sampling mechanism for any kind of Monte Carlo method, such as the "stochastic diagonalization" [11], due to its ability to identify the most important configurations contributing to the structure of the low-lying state. It may also be applied to more general calculations such as those for atoms, molecules, or atomic clusters.

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