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Unrestricted symmetry-projected Hartree-Fock-Bogoliubov calculations for some PF-shell nuclei

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Abstract. Total binding energies and yrast energy spectra of three selected 1p0f–nuclei have been calculated using an unrestricted Hartree–Fock–Bogoliubov approach with symmetry–projection before the variation. The full 1p0f–shell has been used as single–particle basis and the semi–empirical FPD6 interaction as effective Hamiltonian. The results are compared to those of truncated shell–model calculations performed with the OXBASH code. In the middle of the 1p0f–shell the variational method yields energy gains up to 4.5 MeV and thus proves to be far superior than the conventional truncation methods at least if in the latter only up to about 13000 configurations for each spin–isospin combination are admitted.

1 Introduction

With the two assumptions that

(1) a finite number of single particle orbits around the Fermi–level is a sufficiently large model space to compute the properties of the ground and low excited states of a considered nucleus and
(2) for this model space an appropriate effective Hamiltonian is known

the nuclear many–body problem can be solved exactly, at least in principle. Because of the finite number of single particle orbits the number of possible A–nucleon configurations is finite, too, and thus, if the Hamiltonian is known, it can be diagonalized in the resulting complete space. This is done in conventional nuclear shell–model configuration–mixing (SCM) calculations. Unfortunately, the number of A–nucleon configurations to be treated increases dramatically with the number of single particle orbits included in the model space as well as with the number of valence nucleons. Thus complete SCM calculations up to now have been restricted to rather small model spaces. For a long time these were of the size of the 1s0d–shell. Recently, however, with the tremendous improvement in computer facilities, also conventional SCM calculations within a full 1p0f–basis have become possible at least up to $A \sim 56$ [1]. To tackle the problem of even larger dimensions stochastic quantum Monte Carlo approaches, like the shell–model Monte Carlo (SMMC) [2] or the quantum Monte Carlo diagonalisation (QMCD) [3], as well as conventional approximative truncation methods [4,5] have been used.

An alternative to these methods is the use of variational techniques on the basis of much fewer but more complicated configurations like, e.g., symmetry–projected generalized Slater–determinants of the Hartree–Fock–Bogoliubov (HFB)–type. These techniques avoid a truncation of the shell–model configuration space "by hand" as in the conventional or by "throwing dice" as in the Monte–Carlo methods but leave the selection of the relevant degrees of freedom entirely to the chosen Hamiltonian itself. Furthermore, they have the advantage that they can be used also in rather large model spaces including two or even three major shells which are out of reach of the SCM approach even on modern computers. Several methods along these lines have been developed within the last decade [6-8]. The simplest of them is the so–called VAMPIR (**V**ariation **A**fter **M**ean–field **P**rojection **I**n **R**ealistic model spaces)[6-11] approach which approximates each of the yrast–states of a considered nucleus by a single symmetry–projected HFB vacuum with the underlying mean–fields being determined by independent variational calculations. Additional correlations within some yrast–state can then be accounted for by adding successively in a chain of variational calculations additional symmetry–projected HFB configurations. This is done in the FED (i.e., **FE**w **D**eterminants) VAMPIR approach [12]. The first excited state with the same symmetry as a certain yrast state can be described by eliminating the VAMPIR (or FED VAMPIR) solutions from the variational space by Gram–Schmidt–orthogonalisation and then determining the optimal one– (or few–) determinant solutions for this first excited state. Afterwards, this solution can be

eliminated from the variational space, too, and the second excited state can be calculated and so on, up to the desired number of excited states with the same symmetry has been reached. Finally, the residual interaction between all these solutions is diagonalized. This procedure is used in the EXCITED VAMPIR, which allows for only one symmetry–projected determinant per state, and its extension the EXCITED FED VAMPIR approach, which admits several of them per considered state [11-13].

Obviously, these chains of rather sophisticated variational calculations cannot be performed ad infinitum. They will definitely be limited to the lowest few states with particular quantum numbers. If one is interested in the whole excitation spectrum of the nucleus with respect to a particular (e.g., electromagnetic) operator, one is therefore forced to simplify the procedure. One way to do this is to expand the wave functions for a given symmetry around the corresponding VAMPIR solution as it is done in the MONSTER (**MO**del handling many **N**umber and **S**pin projected **T**wo quasi–particle **E**xcitations in **R**ealistic model spaces) approach [6,14], which (for a given symmetry) diagonalizes the chosen Hamiltonian in the space of the VAMPIR solution and all the symmetry–projected two–quasi–particle excitations with respect to it.

Within the last fifteen years all these methods have been applied rather successfully to many nuclear structure problems (see, e.g., the reviews [6,11,15]). For example, they have been used rather extensively for the theoretical investigation of shape coexistence, shape transitions [16,17] and proton–neutron pairing correlations [18] in the $A \sim (70-80)$ mass–region nuclei.

However, out of numerical reasons, all these applications have still been restricted by assuming at least time–reversal and axial symmetry for the underlying HFB vacua. Only recently these approximations could be removed and completely unrestricted "General Complex VAMPIR" (GCV) calculations have been reported for selected nuclei within an 1s0d–shell basis [19]. It turned out that the energies of the "exact" SCM yrast spectra of these nuclei could be extremely well reproduced using only one symmetry–projected HFB configuration per state.

In the present paper we shall report the results of such unrestricted calculations for ^{46}Ti, ^{50}Cr and ^{62}Zn. Again we shall use only the one–determinant VAMPIR approach, which is the simplest of the variational methods mentioned above. We did not, however, impose any symmetry restrictions on the underlying HFB vacua. Yrast spectra and total binding energies will be compared to exact shell–model results, where those are available, otherwise to those of conventionally truncated shell–model calculations. In addition comparison will be made with the experimental data and with the results of the older, more restricted versions of the VAMPIR and MONSTER approaches. Furthermore, the possibilities of using GCV method in even larger model spaces than the 1p0f–shell will be discussed.

We shall start by summarizing the essential features of the GCV model in the next section. A detailed formulation can be found in several publications [8,10,11,12,13,19]. In Sect. 3 we then present and discuss the results. Finally conclusions and an outlook will be given in Sect. 4.

2 The general complex vampir approach

Be $\{|i>,|k>,...\}_{M_b}$ a finite M_b –dimensional set of orthonormal spherical single nucleon states. The corresponding creation and annihilation operators will be denoted by $\{c_i^\dagger, c_k^\dagger, ...\}_{M_b}$ and $\{c_i, c_k, ...\}_{M_b}$, respectively. They fulfill the usual anticommutation–relations for Fermion field operators. The particle vacuum $|0>$ is defined by $c_i|0> \equiv 0$ for all $i = 1, ..., M_b$.

We now introduce quasi–particle creators and annihilators via

$$a_\alpha^\dagger \equiv \sum_{i=1}^{M_b} (A_{i\alpha} c_i^\dagger + B_{i\alpha} c_i) \tag{1}$$

and hence

$$a_\alpha = \sum_{i=1}^{M_b} (B_{i\alpha}^* c_i^\dagger + A_{i\alpha}^* c_i) \tag{2}$$

respectively. (1) and (2) can be combined to a single matrix–equation

$$\begin{pmatrix} a^\dagger \\ a \end{pmatrix} = \begin{pmatrix} A^T & B^T \\ B^\dagger & A^\dagger \end{pmatrix} \begin{pmatrix} c^\dagger \\ c \end{pmatrix} \equiv F \begin{pmatrix} c^\dagger \\ c \end{pmatrix} \tag{3}$$

with F being a $(2M_b \times 2M_b)$–dimensional matrix. In order to ensure anti–commutation relations for the quasi–particle operators (1) and (2) this matrix has to be unitary

$$F F^\dagger = F^\dagger F = \mathbf{1}_{2M_b} \tag{4}$$

Equations (3) and (4) define the famous HFB transformation [20]. It is the most general linear transformation conserving the anti–commutation relations, which can be constructed within the chosen finite single particle basis.

The vacuum $|F>$ for the quasi–particle annihilators (2) is defined by

$$a_\alpha |F> \equiv 0 \quad \text{for} \quad \text{all} \quad \alpha = 1, ..., M_b \tag{5}$$

and may be represented as

$$|F> = \Big(\prod_{\alpha=1}^{M_b'} a_\alpha \Big) |0> \quad \text{with} \quad M_b' \leq M_b \tag{6}$$

where the product runs over all α with $a_\alpha|0>$ being different from zero.

Since the transformation (3) sums over all the quantum numbers characterizing the single particle basis states (isospin–projection, orbital angular momentum, total angular momentum, the 3–projection of the latter, and the radial excitation), $|F>$ is neither an eigenstate of the square of the total angular momentum operator $\hat{I}^2$ nor of its 3–component $\hat{I}_z$. Furthermore particle number and charge conservation are violated and, in general, the vacuum (6) has no definite parity either. The only symmetry

still conserved is the so–called "number–parity" [21], i.e. $|F>$ contains either only components with even or with odd total nucleon numbers A.

From the vacuum (6) one can construct configurations with the desired symmetry quantum numbers $s \equiv AT_zI^\pi$ using the operator [7]

$$\hat{\Theta}^s_{MK} \equiv \hat{P}(IM;K)\hat{Q}(2T_z)\hat{Q}(A)\hat{p}(\pi) \quad (7)$$

Here

$$\hat{p}(\pi) \equiv \frac{1}{2}(1+\pi\hat{\Pi}) \quad (8)$$

with $\hat{\Pi}$ being the parity operator, projects onto definite parity π.

$$\hat{Q}(A) \equiv \frac{1}{2\pi}\int_0^{2\pi} d\varphi exp\{i\varphi(A-\hat{A})\} \quad (9)$$

with $\hat{A}$ being the nucleon number operator, restores the desired total nucleon number A [22], and

$$\hat{Q}(2T_z) \equiv \frac{1}{2\pi}\int_0^{2\pi} d\chi exp\{i\chi(N-Z-\hat{N}+\hat{Z})\} \quad (10)$$

with $\hat{N}$ and $\hat{Z}$ being the neutron and proton number operators, respectively, selects the components with a definite total isospin-projection $2T_z = N - Z$.

Finally

$$\hat{P}(IM;K) \equiv \frac{2I+1}{8\pi^2}\int^{(4\pi)} d\Omega D^{I^*}_{MK}(\Omega)\hat{R}(\Omega) \quad (11)$$

with $\hat{R}(\Omega)$ being the usual rotation operator [23] and $D^I_{MK}(\Omega)$ denoting its representation in angular momentum eigenstates constructs from the $I_3 = K$ component in the symmetry–breaking "intrinsic" frame of reference a configuration in the laboratory frame with total angular momentum I and 3–component $I_z = M$ [24].

Via the K–quantum number the configuration obtained by acting with the operator (7) on the HFB vacuum (6) does still depend on the orientation of the intrinsic quantisation axis. This unphysical dependence is eliminated by taking the linear combinations

$$|\phi_\rho; sM> \equiv \sum_{K=-I}^{+I} \hat{\Theta}^s_{MK}|F> f_{K;\rho} \quad (12)$$

as physical configurations. Even if only a single determinant is considered, the restoration of the rotational symmetry thus introduces additional configuration–mixing coefficients f, which together with the intrinsic degrees of freedom of the underlying HFB transformation will have to be determined by variation.

In the following we shall restrict ourselves to test wave functions of the form (12). However, the extension to linear combinations of several configurations of this type is straightforward [12] and the code we have constructed can handle also this general option. Details of the procedure to determine the underlying mean fields and the configuration mixing by chains of variational calculations are discussed in the [7,12].

In a given basis the unrestricted, complex transformation F mixes all m–states with $m = -j_{max}$ to $+j_{max}$ regardless of parity and proton or neutron origin. Thus after projection of parity, nucleon numbers, and finally the 3–dimensional projection of the total spin any type of state can be described in doubly–even, doubly–odd and odd nuclei already via a single determinant. This is not the case in the older versions of the approach where certain symmetries were imposed on the underlying HFB transformations.

The requirement of axially symmetric HFB transformations induces that the vacua are eigenstates to the 3–component of the total angular momentum operator $\hat{I}_3$ with eigenvalues $K = 0$. The assumption of time–reversal invariance introduces in addition a two–fold degeneracy into the system. Consequently, the resulting test wave functions are restricted to even nucleon number and can only describe states of doubly–even or doubly–odd nuclei. Furthermore, not even all states in these nuclei are accessible. Though by the use of essentially complex transformations all possible two–nucleon couplings are included, particular four– and more–nucleon couplings are missing [7,10,13] : two natural (or unnatural) parity pairs cannot be coupled to an unnatural parity four nucleon wave function and one natural and one unnatural parity pair not to a natural parity four nucleon state. Hence, e.g., out of all the $(0d_{5/2})^4$ shell–model configurations just one $I^\pi = 3^+$ and one $I^\pi = 5^+$ state (both with total isospin T=0) are missing. Similarly, from all the $(0d_{5/2})^6$ configurations one 4^+ and one 6^+ state cannot be accounted for. Consequently, excitations which are dominated by configurations containing such "missing couplings" as irreducible substructures cannot be described even within the COMPLEX VAMPIR approach.

In earlier calculations we had imposed even more severe symmetry restrictions on the HFB transformations : proton–neutron– and parity–mixing were forbidden and only real mean fields were admitted. Consequently, only natural parity states in doubly–even nuclei were accessible by the various so called REAL VAMPIR approaches.

It should be stressed, however, that at least some of these deficiencies can be overcome even on the basis of symmetry–restricted transformations. This is done in the MONSTER approach, a multi–configuration method, which diagonalizes the Hamiltonian in the space of the VAMPIR solution and all the corresponding symmetry–projected two–quasi–particle excitations. In this way, K–mixing is included right from the beginning and missing couplings are avoided. Similar calculations, though on the basis of fixed intrinsic mean fields and restricted to separable forces, have been performed by Hara and Sun [25]. The MONSTER approach, however, is only suited for exited states whose structure is not too different from that of the underlying HFB vacuum.

Table 1. The dimensions of various J^π states for complete and truncated 1p0f–shell SCM calculations are presented. The first column from the left gives the complete shell model configuration spaces for the $T = 1$ states in ^{46}Ti, the next two columns the complete and truncated configuration spaces for the $T = 1$ states in ^{50}Cr. The next two columns present the corresponding numbers for the nucleus ^{62}Zn. The truncation schemes are discussed in the text. Furthermore the table gives the number of variational degrees of freedom included in the GENERAL COMPLEX VAMPIR (GCV), COMPLEX VAMPIR (CV) and REAL VAMPIR (RM) approaches and, for the last two cases, the numbers of configurations included in the COMPLEX MONSTER (CM) and REAL MONSTER (RM) calculations

J^π	^{46}Ti	^{50}Cr	^{50}Cr(T)	^{62}Zn	^{62}Zn(T2)	GCV	CM	CV	RM	RV
0^+	1 514	134 361	800	9 115 163	2 359	1 560	121	120	41	40
1^+	4 105	387 477	2 196	26 632 734	6 626	1 562	337	120	72	40
2^+	6 338	604 907	3 530	42 172 869	10 057	1 564	521	120	139	40
3^+	7 533	763 543	4 436	54 631 847	12 035	1 566	647	120	148	40
4^+	8 026	857 287	5 107	63 333 830	12 637	1 568	727	120	189	40
5^+	7 532	881 146	5 281	67 946 333	11 833	1 570	763	120	176	40
6^+	6 606	846 273	5 216	68 620 892	10 149	1 572	779	120	201	40
7^+	5 223	762 983	4 762	65 804 605	7 908	1 574	781	120	180	40
8^+	3 896	651 241	4 197	60 265 145	5 673	1 576	781	120	201	40

3 Results and discussions

Unlike the 1s0d–space, where complete SCM diagonalisations could be performed already more than 20 years ago, such calculations in a full 1p0f–basis are still a big challenge, though in the meantime dimensions up to about 10 to 20 million configurations can and have been treated within the conventional shell–model [1,26]. So, e.g., Caurier *et al.* [27] reported recently on SCM calculations within a 1p0f–basis with typically as many as 10 million configurations. However, for nuclei in the middle of the shell like e.g. ^{62}Zn, even these large dimensions do not span the complete space. It is therefore an interesting question, how the above mentioned variational methods perform with respect to the truncated SCM. For this purpose we decided to perform GCV calculations for the yrast spectra of the three nuclei ^{46}Ti, ^{50}Cr and ^{62}Zn in the full 1p0f–basis and to compare the results for the energies with those of complete and truncated SCM calculations as well as to those of the older, symmetry–restricted versions of the VAMPIR and MONSTER approaches. Note, that the VAMPIR approach describes each yrast state by a single symmetry–projected HFB determinant instead of using thousands or even millions of configurations.

Unfortunately, the modern SCM codes were not available to us. Instead we used the OXBASH code [28] which was not designed to treat particularly large dimensions so that here much more severe truncations than mentioned above were necessary. In fact because of the limited computer facilities we used we had to keep the SCM dimensions for each angular momentum and isospin JT below ~ 13000. As can be seen from Table 1, which displays the complete SCM dimensions for the three considered nuclei, this is more than sufficient for ^{46}Ti so that there the SCM results are "exact". For ^{50}Cr we truncated the number of configurations by limiting the number of 0f7/2–nucleons to a minimum of 7 and a maximum of 10 and allowing maximally only 3 nucleons in the 1p3/2– and only 2 nucleons in the 0f5/2– and 1p1/2–levels, respectively. Finally, for ^{62}Zn two different truncations were used. In the less severe of them (T2) maximally 2 holes in the 0f7/2–orbit were admitted and only 0 to 8 nucleons were allowed in its spin–orbit partner, while the 1p3/2– and 1p1/2–occupations were not restricted. This yields the dimensions listed in the 6-th column of Table 1. The stronger trucation (T1) (not displayed in the table) allowed for maximally 1 hole in the 0f7/2–level, and limited the 0f5/2– and 1p3/2–occupations to 0 to 5 and 2 to 7, respectively, while again no restriction was made for the number of nucleons in the 1p1/2–orbit.

Furthermore Table 1 displays the number of variational parameters obtained for the "real" (RV), "complex" (CV) and "general complex" (GCV) VAMPIR approximations and, for the first two of those, the number of configurations used in the corresponding MONSTER calculations. Note, that in the GCV case the number of variational variables increases with the total angular momentum. This is due to the additional variational degrees of freedom f introduced in (12). The increase of the MONSTER dimensions with increasing angular momentum is due to the inclusion of the two–quasi–particle configurations with $K \neq 0$. It is clearly seen, that (except for the 0^+ in ^{46}Ti) even in the GCV approach the number of variational degrees of freedom is considerably smaller than the dimensions of the SCM configuration spaces though the latter had been severly truncated in the two heavier nuclei.

As effective interaction we used for all calculations the Hamiltonian FPD6 described in detail in [29]. This semi–empirical interaction is based on a parametrization in terms of density–dependent one–boson exchange potentials with 18 parameters which were fitted in the above mentioned reference together with the single particle energies using the OXBASH code to a selected set of 61 energy levels in nuclei in between ^{41}Ca and ^{49}Ca.

Figure 1 displays the binding energies relative to the ^{40}Ca core for the yrast spectrum of ^{46}Ti up to spin 8^+ as obtained by various versions of the VAMPIR and MONSTER approaches. The results are compared to those of

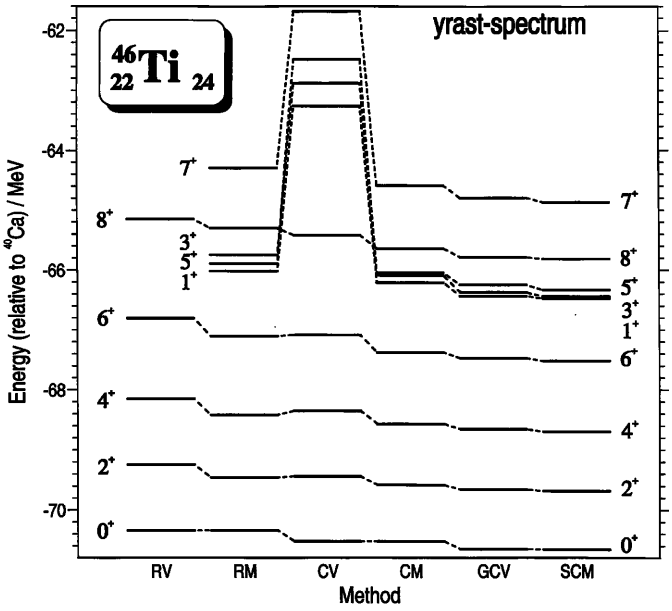

Fig. 1. The yrast spectrum of the nucleus ^{46}Ti as obtained with different variational methods discussed in the text are compared to that resulting from a complete shell–model diagonalisation

a complete shell–model diagonalisation (SCM) which are presented in the rightmost column of the figure. Starting from the left we first give the results of REAL VAMPIR (RV) calculations. In this approach axial and time–reversal symmetry are imposed on the underlying HFB transformations, proton–neutron mixing is neglected and only real HFB transformations are admitted. As a consequence of these symmetry–restrictions, only states with even spin and positive parity in doubly even nuclei can be described. As can be seen, already in this simple approach, the relative excitation energies are not far from those of the SCM spectrum, the differences in absolute energy, however, are larger than 300 keV for all states. Performing a REAL MONSTER (RM) calculation on top of the REAL VAMPIR vacuum for the ground state gives slightly more binding, except for the ground state which, as a variational solution, is energetically stable against the symmetry–projected two–quasipartile admixtures and thus remains unchanged. Note, that because of the inclusion of time–reversal non–invariant configurations the odd spin states can be described in the RM approach, too. The quality of their description is about equally good as for the even spins, though the order of the nearby 3^+ and 5^+ states is inversed with respect to the SCM spectrum.

The third column presents the result of the COMPLEX VAMPIR (CV) approach. Here proton–neutron mixing is allowed and essentially complex HFB transformations are admitted. Thus, even assuming still time–reversal and axial symmetry, now all possible time–even as well as time–odd two–nucleon couplings are accounted for. However, as already mentioned above, some 4– and more nucleon–couplings are missing in this approach. Thats why the inclusion of the additional correlations does improve the even spin states obtained in the RV (and RM) approaches, the odd spin states, however, calculated within the CV approximation suffer from these missing couplings and are more than 2 MeV off from the exact results. The COMPLEX MONSTER (CM) (based on top of the CV ground state solution) leaves again the ground state unchanged, improves, however, on the excited states. The odd spin states are now desribed equally well so that all the states displayed here are only about 200 KeV less bound than the SCM results.

Finally, the results of the unrestricted GENERAL COMPLEX VAMPIR (GCV) approach is presented in the fifth column. Though here each state is approximated by only one symmetry–projected determinant, the agreement with the exact SCM results is here even better than in the CM calculation. All the considered states are now less than 100 KeV above the exact results and the ground state is even exact. This can be understood from the fact that for spin–parity 0^+ the number of variational degrees of freedom is slightly larger than the corresponding SCM dimension as can be seen from Table 1. The remaining differences for the higher spin states could be easily removed by correlating the GCV solutions with one or two additional symmetry–projected determinants as indicated in the last chapter. We can conclude that inspite of the much larger model space at least at the beginning of the 1p0f–shell the agreement of the one–determinant GCV approach with the exact SCM results for the yrast states is equally good as throughout the 1s0d–shell which had been considered in an earlier paper [19]. Finally, we would like to stress that a GENERAL COMPLEX MONSTER (GCM) [30] calculation would not change the GCV yrast spectrum at all. Because of the absence of any symmetry–restrictions the GCV solutions are now energetically stable against admixtures of arbitrary symmetry–projected two–quasi–particle excitations and not only of those with $K = 0$ as it was the case in the RM and CM approaches. Thus (if based for each spin on the corresponding GCV solution) the GCM approach can only reproduce the GCV yrast states.

As next example we considered the yrast states of the nucleus ^{50}Cr. The results are displayed in Fig. 2. Rather similar features as in case of ^{46}Ti are observed as, e.g., the bad description of the odd spin states by the CV approach due to the missing couplings and its improvement in the CM approximation. The latter was here obtained by using for each angular momentum that particular CV solution for the even spin states states which yielded after diagonalisation the lowest energy for the corresponding yrast state. As expected because of the larger configuration space the energy gains of the unrestricted GCV approach with respect to the CM spectrum are here considerably larger than for the Titanium nucleus. The various VAMPIR and MONSTER results are compared here to a severly truncated SCM calculation (see Table 1). The severe truncation has the consequence that the resulting yrast states are even less bound than in the simple RV approximation (at least up to angular momentum 4^+) and considerably less bound (up to about 2.5 MeV) with respect

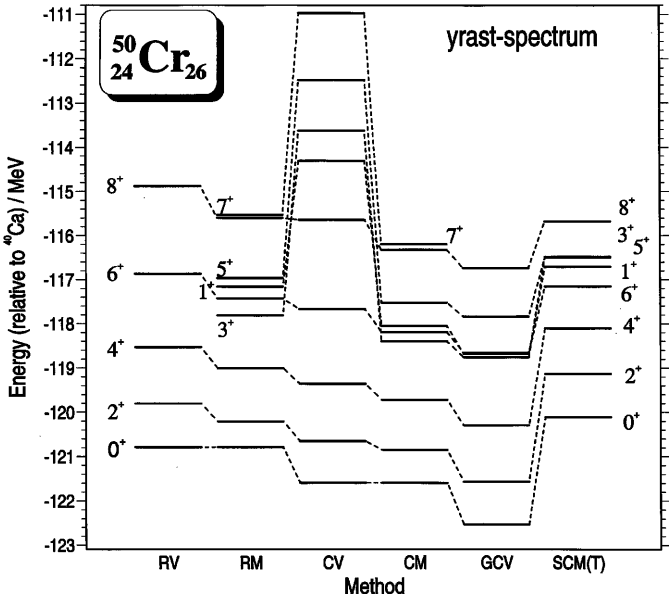

Fig. 2. Same as in Fig.1, but for the nucleus ^{50}Cr. Here the shell–model configuration space has been severly truncated as explained in the text

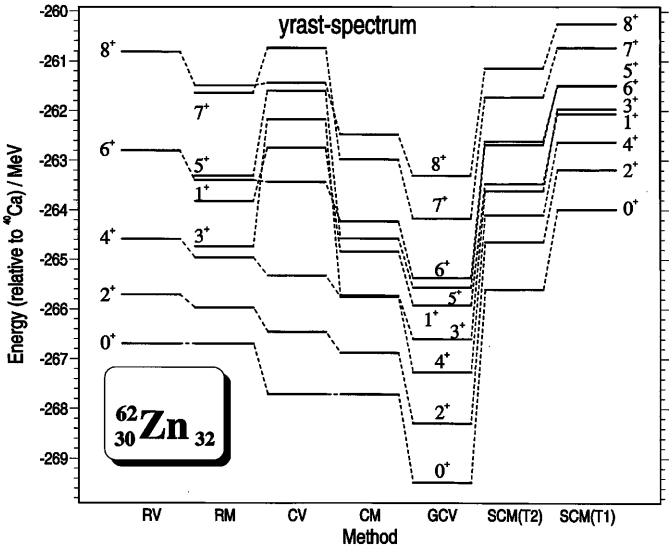

Fig. 3. Same as in Fig.1, but for the nucleus ^{62}Zn. The details of the two conventional shell–model truncation schemes are given in the text

to the GCV spectrum. Obviously, this comparison is not quite fair, since ^{50}Cr can be done exactly by more modern shell–model codes [1]. Using the same force such calculations would obviously obtain more binding then the one determinant GCV approach. However, the example shows clearly, that with respect to severe conventional truncations, the variational method is clearly preferable.

Finally, we consider the nucleus ^{62}Zn. Table 1 shows that here even modern shell–model calculations have to be truncated. Because of the use of the OXBASH code and of the limited computer power available to us we used again rather severe truncations. Only up to about 13000 configurations for each spin–isospin combination were admitted in the truncation nr. 2 (T2) and for comparison in addition even a more severe truncation (T1) was used. The results of these calculations are displayed in Fig. 3. In the various versions of the VAMPIR and MONSTER approaches again rather similar features as in case of ^{46}Ti and ^{50}Cr are observed, however, here the energy gains of, e.g., the CV spectrum with respect to the RV results are much larger. This indicates the presence of more time–odd correlations in this nucleus than in the other two. Even larger are the energy gains of the unrestricted GCV approach with respect to the CV and also CM results which again for each angular momentum were based on that even spin CV solution which yielded the minimal CM yrast energy. As compared to the truncated SCM spectra, the GCV approach yields energy gains of about 4 MeV with respect to the truncation T2 and even about 5.5 MeV with respect to the more severe truncation T1. Thus, even more than in the nucleus ^{50}Cr the unrestricted one–determinant GCV approach seems to provide a much better truncation scheme than the conventional SCM truncations at least if the latter are rather severe.

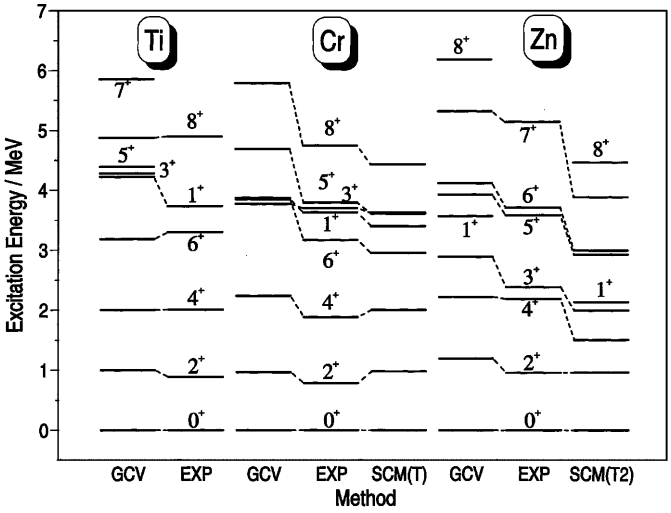

Fig. 4. The one–determinantal GCV yrast spectra of the nuclei ^{46}Ti, ^{50}Cr and ^{62}Zn compared to the experimental energy levels [23]. For the latter two nuclei the results of the truncated shell–model calculations are presented, too

Figure 4 compares the GCV and the truncated SCM results to the experimental spectra [31]. Unlike in the previous figures here only the relative excitation energies are plotted. In the nucleus ^{46}Ti the complete SCM calculation and the GCV approach differ in the average by less than 100 KeV. Thats why here only the GCV spectrum is shown. The experimental levels are reproduced rather well in this nucleus. This is somehow to be expected since the chosen effective Hamiltonian was optimized to energy levels in this mass region. In ^{50}Cr, the truncated shell–model spectrum is considerably more compressed than the GCV one and agrees better with the experimental data. However, one has to keep in mind, that the GCV levels are all considerably more bound than the truncated SCM

Table 2. The total binding energies (in MeV) relative to the ^{40}Ca core, including the Coulomb corrections, are presented. The results of the GCV approach and of the complete shell–model calculations in ^{46}Ti and the truncated ones in the two other nuclei are compared to experimental values

^{Z}A	BE(Exp.)	BE(SCM)	Δ(SCM)	BE(GCV)	Δ(GCV)
^{46}Ti	56.14	55.90	−0.24	55.90	−0.24
^{50}Cr	92.99	89.88	−3.11	92.30	−0.69
^{62}Zn	196.07	184.75	−11.32	188.63	−7.43

ones. Furthermore, no T=1 states in this mass region have been used to fix the effective Hamiltonian. Thus this better agreement has to be taken with care. It is rather likely to be accidental. In ^{62}Zn we observe again that the (less severe) truncated SCM spectrum is considerably compressed with respect to the GCV results. Here, however, the latter agree better with the experimental findings, especially for the higher spin states like 4^+, 5^+, 6^+ and 7^+. Unfortunately, again the better agreement of one of the methods with the experimental data should be taken with care. The Hamiltonian has not been fitted in this mass region.

Obviously, it would be interesting to see how the GCV approach (and its improvements like the GENERAL EXCITED FED VAMPIR approach) would perform with respect to less severly truncated shell–model calculations like, e.g., those of Caurier *et al.* [27] who used a different interaction. We intend to do such comparisons in a forthcoming paper.

Finally, we would like to compare the total binding energies obtained for the ground state of the three considered nuclei with the experimental data [32]. For this purpose we have to correct the latter for the Coulomb interaction which was not included in the calculations. These Coulomb corrections can be estimated from the differences in binding energies between pairs of analog states (see [29,33]) and are listed in [34]. For ^{62}Zn unfortunately, there is no entry in [34]. Thus, for this nucleus we used an approximate formula for the Coulomb correction with the parametrisation of Caurier*et al* [1] based on a fit for nuclei between $A = 42 - 64$:

$$E_C = 7.44 \times p + 0.137 \times p(p-1) - 0.049 \times pn \qquad (13)$$

where p and n denote the numbers of valence protons and neutrons, respectively. The results for the total binding energies are displayed in Table 2.

As can be seen, the experimental binding energy for ^{46}Ti is nicely reproduced. For ^{50}Cr the error of the GCV binding energy is still only 0.7% while in the middle of the shell, for ^{62}Zn, it deviates by 3.8% from the experimental value while for the truncated SCM the deviations in these two nuclei are considerably larger. Again, however, one has to be a little careful with this comparison, since the chosen effective Hamiltonian was not optimized for the latter two nuclei and since for the SCM calculations rather severe truncations have been used.

4 Conclusions

In the present paper we have reported results of completely unrestricted symmetry–projected HFB calculations to three selected nuclei in a full 1p0f–shell basis. The results of these "GENERAL COMPLEX VAMPIR" (GCV) calculations have been compared to those of earlier, more restricted versions of the same approach as well as to those of multi–configuration approaches based on the corresponding mean fields (MONSTER) and to those of exact and conventionally truncated shell–model diagonalisations (SCM).

It turned out that at the beginning of the shell (as example here the nucleus ^{46}Ti was considered) the "exact" shell–model energies for the yrast states can be reproduced rather well even using only one symmetry–projected HFB determinant per state. The deviations are for all considered states less than about 100 KeV. For heavier systems (here the examples ^{50}Cr and ^{62}Zn have been considered) the variational GCV method is far superior than the conventionally truncated SCM approach. Here the GCV yrast states are more bound than the corresponding truncated SCM ones by about 2.5 and 4 MeV, respectively. Obviously, one has to stress that in the SCM diagonalisations here only about up to 13000 configurations for each spin–isospin combination have been included. Nowadays the conventional SCM method can treat up to about 10 to 20 million configurations and thus yields "exact" results for 1p0f–shell nuclei up to about $A \sim 56$. However, one has to keep in mind, too, that the GCV approach uses only one symmetry–projected determinant per state and is hence essentially a "free" theory. It can be easily improved by adding successively a few correlating configurations in a chain of variational calculations. Thus the results presented here clearly prove that the variational method provides an excellent tool to truncate shell–model spaces in a very effective way.

Obviously, wherever complete SCM diagonalisations are possible they are preferable with respect to the variational approaches discussed here. One cannot be more exact than exact. However, this is not what, e.g., the GCV approach is designed for. VAMPIR and MONSTER are alternatives for such model spaces where SCM calculations are only possible in either severely truncated model spaces or cannot be done at all within an acceptable truncation scheme. This includes almost all problems where model spaces including more than one major shell are needed, e.g., even comparatively simple problems like the desription of negative parity states in 1s0d–shell nuclei. These are the kind of problems the approaches discussed here are aiming at.

On the other hand, as soon as the basis becomes larger than a single major shell, we encounter a well known though rarely discussed problem. Most approaches to the nuclear many body problem (including the SCM and the various VAMPIR and MONSTER approaches) expand the wave functions in terms of Slater or generalized Slater determinants. In this way the Pauli principle is fulfilled by construction but Galilei–invariance is severely broken. It is usually argued that this is an 1/A effect and thus of mi-

nor importance at least for systems heavier than ^{16}O. Recent investigations [35,36] show that this statement is not true. Spectroscopic factors, form factors, response functions and even energies can be severly affected by an incorrect treatment of the center of momentum motion even in nuclei like ^{40}Ca and beyond. We therefore believe that the restoration of full Galilean invariance, obviously before the variation, is unavoidable.

This can be achieved again by projection methods [35,36]. The corresponding integral operator involves another three–fold integration to be performed in addition to the five–fold integration already present in the GCV approach. Thus a correct treatment of Galilei–invariance is hardly possible on present day sequential or vector computers. For parallel processing the situation is quite different. The GCV calculations involving multi–fold integrations are particularly suited for parallel data processing : test calculations in 1s0d–shell [19] showed a linear increase of the inverse CPU time with the number of processors available and thus the optimal performance which can be reached on parallel computers. Since, furthermore, we have already succeeded in developing the mathematical apparatus needed for the projection of general HFB determinants into the center of momentum rest frame, we are confident that this procedure will become numerically feasible in a not very distant future.

The intensive work on the attempt to implement Galilei–invariance in the GCV approach is also the reason why, as in [19], also here only energies and not other important observables like, e.g., electromagnetic transitions have been calculated. Such observables will be considered at a later stage.

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