Eur. Phys. J. A **2**, 371–377 (1998)

THE EUROPEAN PHYSICAL JOURNAL A

Unrestricted symmetry-projected Hartree-Fock-Bogoliubov calculations for SD-shell nuclei

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Received: 26 February 1998 / Revised version: 8 May 1998
Communicated by D. Schwalm

Abstract. The solution of the Hartree–Fock–Bogoliubov problem with restoration of the broken symmetries before the variation has been generalized for the use of totally unrestricted quasi–particle determinants. With this method doubly–even, doubly–odd and odd nuclei can be treated on the same footing. Comparison with the results of complete shell–model diagonalizations shows that already one–determinant representations yield a very good approximation to the exact solutions even in the middle of the 1s0d shell. The problem is especially suited for numerical implementation on parallel computers. First tests show a linear dependence of the inverse CPU time with the number of processors used.

PACS. 21.10.-k Properties of nuclei, nuclear energy levels – 21.60.Jz Hartree-Fock and random-phase approximation

1 Introduction

Many nuclear structure problems require the use of single particle basis–systems, which are far too large to allow for a complete diagonalization of a suitably chosen effective many–nucleon Hamiltonian, as it is done in the Shell–model Configuration-Mixing (SCM) approach [1]. Obvious examples are the spectra of medium–heavy and heavy deformed nuclei, but even such comparatively simple tasks as the description of negative–parity states in light even A nuclei. For such problems one has therefore to truncate the complete SCM expansion of the nuclear wave functions to a numerically feasible number of A–nucleon configurations without loosing the essential degrees of freedom relevant for the particular states under consideration. A simple truncation of the SCM space according to the unperturbed energies of the configurations is rather questionable. This prescription [2] yields often unsatisfying convergence properties especially for those states in the nuclear spectrum, which are of a more collective nature. We did follow therefore in the last years another avenue, which starts from the ideas of mean–field theory and tries to extract the relevant degrees of freedom directly from the nuclear Hamiltonian via variational procedures. In this way the selection of the configurations is left entirely to the dynamics of the system considered, and the ambiguities of the traditional truncation schemes are avoided.

Out of the various possibilities to explore this avenue [3-5], the VAMPIR (**V**ariation **A**fter **M**ean–field **P**rojection **I**n **R**ealistic model spaces) approach [6,7], its extension for the description of excited states, the EXCITED VAMPIR [5,8], and finally the inclusion of additional correlations via the EXCITED FED VAMPIR method [9] are the most elaborate ones. In the VAMPIR approach the energetically lowest ("yrast") state with a given symmetry (i.e. fixed number of protons and neutrons, definite parity and angular momentum) is approximated by a single symmetry–projected Hartree–Fock–Bogoliubov (HFB) vacuum. The underlying mean–field is determined by a variational calculation after the projection. This yields the optimal description of each yrast–state in a symmetry–projected independent quasi–particle picture. The EXCITED VAMPIR approach is the straightforward extension of this method for the excited states with the same symmetry. Here for the first excited state of the considered system simply a second symmetry–projected HFB vacuum being Gram–Schmidt–orthogonalized to the yrast–solution is taken as test wave function. The variation yields then the optimal description of the first excited state again by a single projected determinant. In the same way afterwards the higher excited states are constructed. Finally the residual interaction is diagonalized in between all these solutions. This procedure has the advantage that one can describe excited states with a structure completely different from that of the corresponding yrast–state.

The EXCITED FED VAMPIR approach uses several instead of only one symmetry–projected HFB vacua for the description of each state. It determines each of the different underlying HFB transformations successively together with the configuration mixing via a chain of variational calculations. In this way it is ensured that each further symmetry–projected determinant does not disturb the wave function more than the last one added previously.

In addition the confidence level of the calculation can be improved considerably. These methods have been applied [10] with good success for example to the rather complex shape–coexistence phenomena in the $A \sim 70$ mass–region. However, even in the most recent versions of these methods we still had imposed time–reversal invariance and axial symmetry on the underlying HFB transformations (see [5] and references therein).

These last restrictions will be removed in the present paper. For the first time we shall report results of symmetry–projected HFB calculations on the basis of completely unrestricted quasi–particle determinants. For simplicity we shall restrict ourselves to the one determinant VAMPIR approach. However, the mathematical formalism as well as its numerical implementation for the more elaborate versions mentioned above are ready for application, too.

In the next section we shall introduce the basic ingredients of the theory. They have been discussed in detail elsewhere [7,8,9] and will hence be sketched only briefly. Section 3 will list the advantages of the new approach with respect to its older, more restricted, versions. Section 4 displays details of the numerical implementation and demonstrates its excellent performance on data–parallel computers. In Sect. 5 we present the results of selected applications in 1s0d–shell nuclei and compare them to the results of exact SCM calculations. Furthermore we discuss the improvements with respect to symmetry–restricted versions of the VAMPIR approach. Conclusions will be drawn and an outlook on improvements necessary for applications in larger model spaces will be given in Sect. 6.

2 Outline of the theory

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. Eqs. (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 $(2M_b * 2M_b)$–dimensional matrix. In order to ensure anti–commutation relations for the quasi–particle operators (1) and (2) this matrix has to be unitary

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

Eqs. (3) and (4) define the famous HFB transformation [11]. 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" [12], 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 $s \equiv A T_z I^\pi$ using the operator [5]

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

Here

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

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

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

with $\hat{A}$ being the nucleon number operator, restores the desired total nucleon number A [13], and

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

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

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

with $\hat{R}(\Omega)$ being the usual rotation operator [14] 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 $I_z = M$ [15].

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

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

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 [9] 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 [5, 9].

3 Unrestricted versus symmetry restricted methods

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 $\hat{I}_z$ 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 [5,7,8] : 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 up to now most advanced COMPLEX VAMPIR approach.

In the 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 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 [16]. The MONSTER approach, however, is only suited for exited states whose structure is not too different from that of the underlying HFB vacuum.

4 Numerical implementation and performance

Since time–reversal invariance is not any more imposed on the HFB transformation there is no a priori two–fold degeneracy in the system. Thus there is no advantage in using the canonical representation as it was done in the earlier versions of the VAMPIR approach. Instead all the matrix elements are now calculated in terms of the A– and B–matrices of the HFB transformation (3, 4). Furthermore, since also axial symmetry is not any more required, the sums run over all the quantum numbers and not only over subspaces with definite value of the 3–component of the intrinsic angular momentum. This in fact makes the numerical implementation simpler than in the previous approaches which made explicit use of the symmetries required. On the other hand the number of linear independent variables in the variation does increase considerably. E.g., in an sd–shell basis, we have 20 variables in the REAL VAMPIR, 56 in the COMPLEX VAMPIR and 552 in the unrestricted approach just for the variation of the HFB–transformation alone. In the unrestricted case we have furthermore to add the configuration (K–) mixing degrees of freedom. For given total angular momentum I these are 2I extra variables (one drops out because of normalisation). For unrestricted calculations in larger basis spaces, the number of variables will easily reach a few thousands and some care has to be taken in choosing the numerical procedure used for the minimisation.

We therefore replaced the Quasi–Newton method used in the older versions of the code (there the inverse Hessian was updated) by a more modern implementation updating the Hessian itself. This method, given by Gill and Murray [17], is equally fast as the old version, however, numerically more stable.

Number parity is still conserved even for general HFB vacua of the form (6). Thus they contain either only components with even or with odd total nucleon number. Obviously one has to ensure the right number parity in the starting wave function for the system under consideration. This is achieved by blocking one orbit if odd A systems are to be described. In this case the calculation of the rotated overlap–matrix is slightly more involved as for the even A–case but still straightforward.

Obviously we pay a price for the use of unrestricted transformations: in the earlier applications two of the three integrations induced by the angular momentum projection could be performed analytically due to axial symmetry. Hence together with the two integrations induced by the projection on good nucleon numbers only three–fold integrations had to be performed. Now also the two rotations around the 3–axis have to be done numerically so that the calculation of energy– and overlap–matrices as well as of the corresponding gradient vectors involves always five–fold numerical integrations.

Such calculations, at least in larger model spaces, can hardly be performed on sequential– or even vector–computers, since the CPU time does increase essentially with the power of number of integrations. On the other hand multi–fold integrations are particularly suited for multi–processor computers. One can distribute the identical mathematical operations to be performed on each grid point combination over the different processors available, collect the results at the end and perform the integration. Since the calculation of the projected matrix elements (overlap, energy and corresponding gradients) is the by far most time consuming part of the program (more than 99 percent), the code can be parallelized almost entirely.

In practice we have achieved this using the Cray Fortran 77 package on the Cray T3D computer in Edinburgh. How nicely this procedure works, can be seen from Fig. 1, where (after subtracting a constant overhead of 10 seconds) the inverse CPU time needed by the unrestricted GENERAL VAMPIR code is plotted as function of the number of processors used. We observe a perfectly linear behaviour which is the optimal performance one can reach in parallel computing.

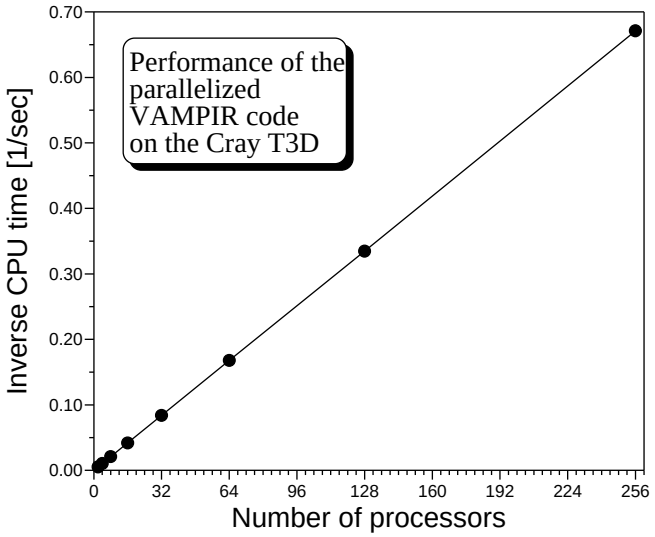

Fig. 1. Performance of the parallelized GENERAL COMPLEX VAMPIR code on the Edinburgh Cray T3D. Plotted is the inverse CPU time versus the number of processors used

5 Results and discussions

The quality of the unrestricted VAMPIR approach which we shall denote as GENERAL COMPLEX VAMPIR (GCV) in the following was tested by selected applications in an 1s0d–shell model space. This allows a direct comparison with exact SCM diagonalizations as well as with the results of earlier more restricted VAMPIR and MONSTER calculations. We chose nuclei out of the middle of the 1s0d–shell where the dimensions of the shell–model configuration spaces are considerably larger than the number of variational variables present in the GCV approach.

The single particle energies ($\epsilon(0d_{5/2}) = -4.15$ MeV, $\epsilon(1s_{1/2}) = -3.28$ MeV, and $\epsilon(0d_{3/2}) = +0.93$ MeV) have been taken from experiment [18]. As effective interaction the mass-dependent version of the Chung and Wildenthal force [19] has been used, except for the fact that the exponent α of the scaling–factor $\hat{V}(A) = \hat{V}(A = 18)(\frac{18}{A})^{\alpha}$ has been chosen as $\frac{1}{3}$ instead of 0.3.

Figure 2 displays the total binding energies relative to the ^{16}O core of the yrast spectrum of ^{24}Mg obtained by 5 different approximate methods and compares them to the exact SCM results presented in the first column from the right. Starting from the left we first give the results of REAL VAMPIR (RV) calculations. Odd spins are not accessible in this approach as discussed in Sect. 3. For the even spin states the RV reproduces the relative excitation energies of the SCM spectrum rather well, however, misses the absolute energy by more than 2.5 MeV. In the next column come the results of the REAL MONSTER (RM) which diagonalizes the chosen Hamiltonian in the space of the RV–vacuum obtained for the 0^+ ground state and all corresponding symmetry–projected two–quasi–particle excitations. By construction therefore the total energy of the 0^+ ground state remains unchanged while the higher spin states get some, though small, contributions from the two–quasi–particle excitations. Furthermore, in this case the symmetry–restrictions of the RV calculation are overcome and the odd spin states can be obtained as well. For them, too, the relative excitation energies of the SCM spectrum can be well reproduced, though the order of the 4^+ and 3^+ excitations is reversed.

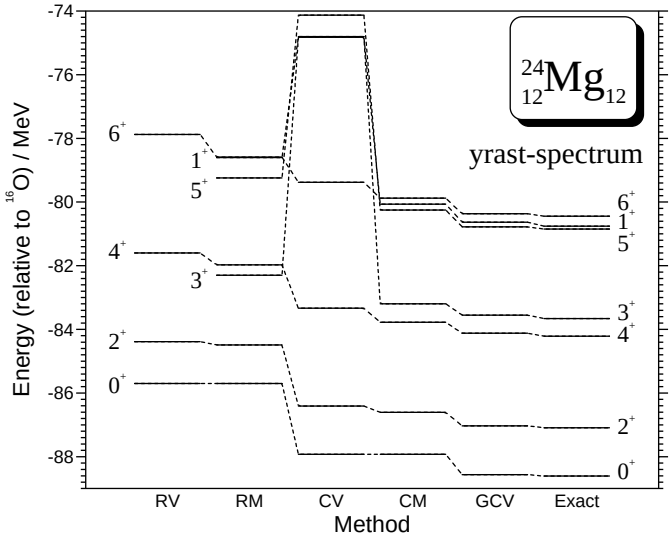

Fig. 2. The yrast spectrum of the nucleus ^{24}Mg obtained with different methods. The various abbreviations are explained in the text

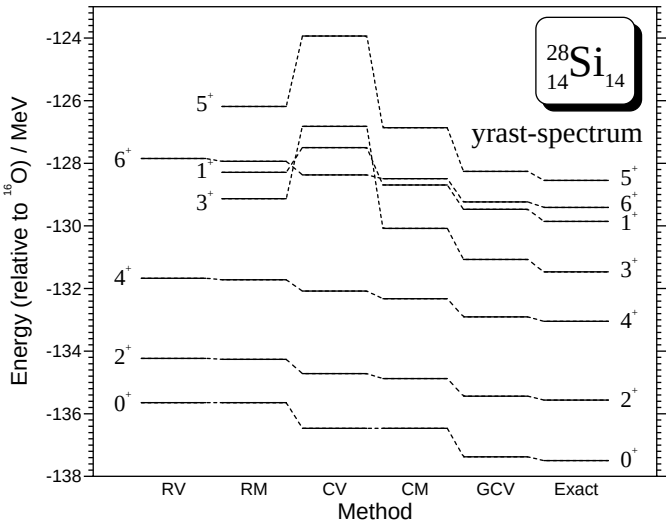

Fig. 3. Same as in Fig. 2, but for the nucleus ^{28}Si

The third column from the left displays the results of the COMPLEX VAMPIR (CV) approach. Here odd spin states can be obtained even from the K=0 vacuum, however, the figure clearly indicates that those states are dominated by four– and more–nucleon couplings which are "missing" in the still time–reversal invariant and axially symmetric vacuum. Thus their description is rather bad. For the even spin states the energy differences are of about the same quality as in the RV calculation, however, the absolute energy is considerably improved with respect to the latter approach : Now the SCM ground state energy is missed by less than 700 KeV. Again the shortcomings for the description of the odd spin states can be overcome by the corresponding multi–determinant COMPLEX MONSTER (CM) approach. Using this method, both, the relative energies of the even and the odd spin states can be reproduced equally well as can be seen in the fourth column from the left which displays the results of [20].

Second but last we show the results of the (one–determinant) GCV calculations. Now not only the relative energies but also the absolute binding energies of both even and odd spin states can be reproduced within about 100 KeV. This is by no means trivial : e.g., the number of SCM configurations for the 3^+ state is 4968 as compared to only 558 linear independent variables in the GCV approach. Note, that the rather complicated SCM expansion of the wave function is in the GCV approximated by a single determinant only. Obviously, the "free" GCV solution could be correlated by additional configurations via the FED VAMPIR method [9]. However, the results presented here clearly demonstrate that there is not much space for such additional correlations at least in ^{24}Mg.

Within the 1s0d–shell the largest SCM dimensions are obtained for ^{28}Si. The results for the yrast states of that nucleus are displayed in Fig. 3. The same methods as in case of ^{24}Mg are compared with each other. We observe a rather similar pattern. Again the GCV results agree well with the SCM spectrum though here the deviations are slightly larger (e.g., about 300 KeV for the 3^+ state which has here 15385 SCM configurations). So, even in the middle of the shell the "free" GCV approach yields an excellent description of the exact solutions.

The same holds for doubly–odd and odd nuclei, too. As an example we present in Fig. 4 the results for the lowest yrast states of the doubly–odd nucleus ^{26}Al. Here no RV results can be given since this method is restricted to doubly–even nuclei only. The RM calculation was based on the RV solution for the ground state of the doubly–even nucleus ^{28}Si. It is seen that also in this case the GCV

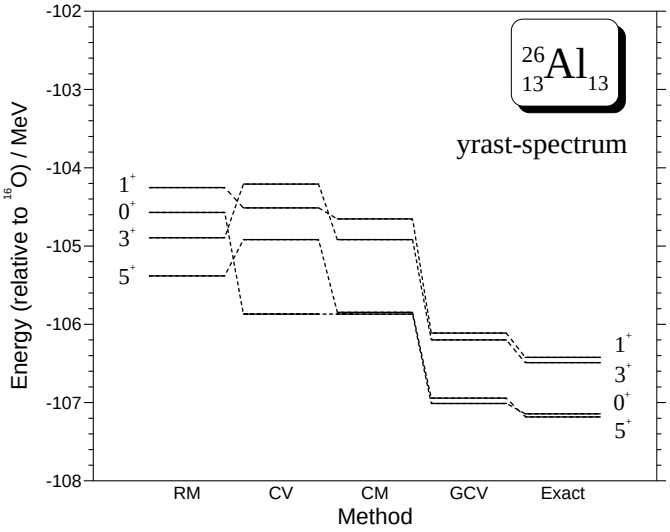

Fig. 4. Same as in Fig. 2, but for the doubly–odd nucleus ^{26}Al. This nucleus is inaccessible in the REAL VAMPIR (RV) approximation. Note the different energy scale as compared to Figs. 2 and 3

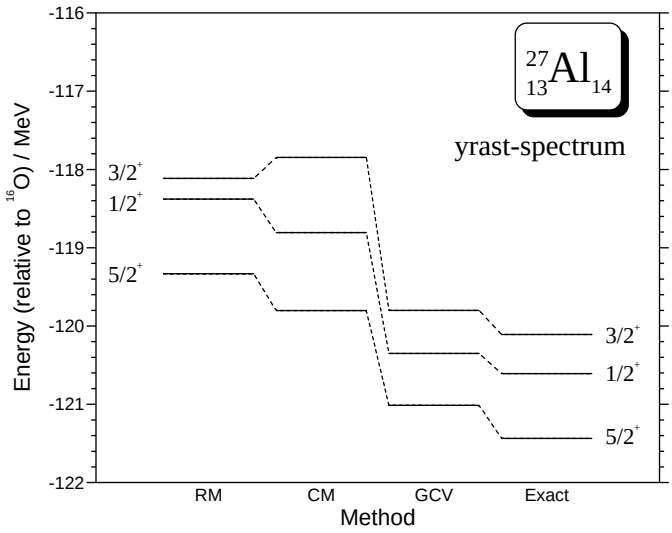

Fig. 5. Same as in Fig. 2, but for the odd nucleus ^{27}Al. Here neither the REAL nor the COMPLEX VAMPIR approach can be used. Again a different energy scale as in Figs. 2 and 3 has been used

approach reproduces the shell–model spectrum very well. However, here remaining differences in absolute energy of about 400 KeV would have to be accounted for by additional correlations. As an example for an odd nucleus we display the results for the three lowest states of ^{27}Al. Because of time–reversal symmetry these states are inaccessible by even the CV approach, so that the GCV spectrum presents the first symmetry–projected one–determinant description of an odd nucleus. Again the agreement with the SCM solutions is excellent. The CM results have been obtained here using only the complete one–quasi–particle configuration space based on the mean–field which was obtained with the CV approach for the 0^+ ground state of the neighbouring doubly–even nucleus ^{28}Si. Thus larger deviations are to be expected for the CM results as in case of the even A nuclei.

6 Conclusions and outlook

In the present paper we have reported results of the first symmetry–projected HFB calculations ever done using entirely unrestricted vacua. Comparison with the results of complete shell–model diagonalizations in an 1s0d–shell basis has shown that the exact results can be reproduced almost perfectly though we have used for each state only a single symmetry–projected determinant, i.e., an essentially "free" theory. This holds even in the middle of the shell where the shell–model dimensions are largest, and furthermore, the agreement is of the same quality for doubly–even, doubly–odd and odd nuclei. Unlike the shell–model, however, the unrestricted GENERAL COMPLEX VAMPIR (GCV) approach is not limited to small model spaces but can be applied in much larger basis systems.

Even in single–shell basis systems complete conventional shell–model calculations become almost impossible above A$\sim$48. So, e.g. in ^{62}Zn already the 0^+–dimension is for a full pf–basis of the order 10^7. As compared with truncated shell–model calculations, allowing for up to 2 holes in the f7/2 orbit, the GCV approach yields here an energy gain of nearly 4 MeV [21]. Full pf-shell calculations, however, are still possible using the modern Monte–Carlo methods [22,23]. Here it would be very interesting to compare the results of such calculations with those of the GCV variational approach.

However, 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 above discussed variational as well as the Monte–Carlo techniques) expand the wave functions in terms of Slater or generalized Slater determinants. In this way the Pauli principle is fulfilled by construction but the Galilean invariance is severely broken. It is usually argued that this is an 1/A effect and thus of minor importance at least for systems heavier than ^{16}O. Recent investigations [24,25] show that this statement is not true. Spectroscopic factors, form factors, response functions and even energies can be severely 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 necessary.

This can be achieved again by projection methods [24]. 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. Similar difficulties are to be expected, e.g., in Otsuka's version of the Monte–Carlo approach [23]. Thus a correct treatment of Galilean invariance is hardly possible on present day sequential or vector computers. For parallel processing the situation is quite different. We have demonstrated in the present study that the multi–fold integrations to be performed in the GCV approach are particularly suited for parallel data processing : we obtained 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.

We are grateful to the experts of the TRACS–project at the Edinburgh Parallel Computer Centre whose advise was essential for the successful numerical implementation of the GCV method.

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