Global microscopic calculations of ground-state spin and parity for odd-mass nuclei

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Systematic calculations of ground-state spin and parity of odd-mass nuclei have been performed within the Hartree–Fock–BCS (HFBCS) approach and the Finite-Range Droplet Model for nuclei for which experimental data are available. The unpaired nucleon has been treated perturbatively, and axial and left-right reflection symmetries have been assumed. As for the HFBCS approach, three different Skyrme forces have been used in the particle-hole channel, whereas the particle-particle matrix elements have been approximated by a seniority force. The calculations have been done for the 621 nuclei for which the Nubase 2003 data set gives assignments of spin and parity with strong arguments. The agreement of both spin and parity in the self-consistent model reaches about 80\% for spherical nuclei, and about 40\% for well-deformed nuclei regardless of the Skyrme force used. As for the macroscopic-microscopic approach, the agreement for spherical nuclei is about 90\% and about 40\% for well-deformed nuclei, with different sets of spherical and deformed nuclei found in each model.

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To describe the rich variety of elementary modes of nuclear excitations and build up some confidence in the approaches used for that purpose, it is important to assess in a quantitative systematic way the quality of the reproduction of experimental static properties. We choose here to compare the results of Skyrme–Hartree–Fock–BCS (hereafter referred to as HFBCS) calculations of ground-state (GS) spin and parity with experimental values assigned with strong arguments available in the Nubase 2003 database\textsuperscript{[1]} for 621 odd-Z and odd-N nuclei. We undertake such a global study with three different effective interactions, namely the SIII \textsuperscript{[3]}, SkM* \textsuperscript{[4]} and SLy4 \textsuperscript{[5]} parameterizations of the Skyrme effective nucleon-nucleon interaction in the mean-field channel, together with a seniority force in the pairing channel. The results are also compared with those obtained previously in the Finite-Range Droplet Model (FRDM)\textsuperscript{[2]}

We would like to emphasize the global character of the present work. Even though some local studies (in limited mass regions) of the GS spectroscopic properties of odd-mass nuclei using such phenomenological interactions have been carried out over the years (see, e.g., Refs.\textsuperscript{[6,7]}), we want to check as completely as possible the relevance of the obtained results by limiting ourselves to two observables, the spin and the parity of the ground state. The present paper is a brief report on these first results. More details on the approximations and technical methods will be given in a forthcoming study of exotic neutron-rich nuclei.

Our self-consistent mean-field approach including pairing correlations relies on the Hartree–Fock and BCS approximations. They have been implemented in earlier fission studies for even-even heavy\textsuperscript{[8,9]} and light nuclei\textsuperscript{[10]} with the Skyrme interaction in its SkM* parameterization which successfully described potential-energy surfaces in terms of constraints on deformation. As for the pairing residual interaction, we use the seniority force in the $T = 1$ channel, neglecting the neutron-proton correlations given the large value of $T_\mu = (N - Z)/2$, and we calculate the strength with a given pairing window in the same approach as the one used by Möller and Nix\textsuperscript{[11]}. In the present study we choose to include in the pairing window all the single-particle states below the Fermi level and those lying $\Delta_{\epsilon} = 6$ MeV at most above the Fermi level. As in Ref.\textsuperscript{[12]} we have included a smooth cut-off as a function of the single-particle state energy with a diffuseness parameter $\mu = 0.2$ MeV.

We assume that GS nuclear shapes possess left-right reflection and axial symmetries. Global studies\textsuperscript{[13,14]} indicate that close to the valley of $\beta$-stability this is true except for a few small regions. Therefore the projection $K$ of the total angular momentum of the nucleus on the $z$-axis, chosen to coincide with the intrinsic symmetry axis, and the parity $\pi$ are good quantum numbers. In mean-field models this also holds for the single-particle states since the mean-field possesses these symmetries. For odd-mass nuclei, the time-reversal symmetry is broken but axial symmetry is assumed to be preserved. Depending on the intrinsic nuclear deformation, different assumptions for the coupling schemes have to be considered.

The nuclei for which the lowest-energy configuration is assumed to be rigid rotors. We can therefore describe the coupling between the unpaired particle and the rotation of the even-even core in the rotor-plus-quasiparticle approximation using HFBCS single-particle states as in Ref.\textsuperscript{[7]}, and we assume that vibrations are “frozen” in the deformed well (zero phonon). To determine the lowest-energy quasiparticle in the HFBCS approach, we use the equal-filling approximation (see Ref.\textsuperscript{[13]} and references quoted therein) to obtain a time-even state having the desired odd number of particles on average and then we create the lowest-energy quasiparticle on this state.

For a spherical nucleus, the GS spin $J$ and parity $\pi$ are assumed to be those of the single nucleon, deduced from the
Calculated GS spin-parity compared to experiment

\[ |\beta_2| \leq 0.01 \text{ or } |\beta_2| \geq 0.10 \]

\[ V_{12} \geq 2 \text{ MeV} \]

FIG. 1: (color online). Comparison with experimental data of the calculated GS spin and parity of odd-mass nuclei for which \( \beta_2 \notin [0.01;0.1] \) and \( V_{12} \geq 2 \text{ MeV} \) throughout the nuclide chart within the HFBCS model using the SIII interaction.

TABLE I: Agreement of GS spin and parity calculated with three different Skyrme interaction in the HFBCS approach and with the FRDM model with respect to Nubase 2003 data \([1]\), for spherical ("Sph.") well-deformed nuclei ("Def.") and all of them ("Total"). For each Skyrme interaction, we indicate in parenthesis on the first line the percentage of agreement obtained when considering either of the two lowest quasiparticles and on the second line the number of nuclei for which the GS spin and parity of the second lowest quasiparticle agrees with the experimental data.

| Model | Sph. | Def. | Total |
|-------|------|------|-------|
| SIII  | 83.9% (90.8%) | 40.5% (61.5%) | 66.4% (79.0%) |
| SkM*  | 76.2% (89.2%) | 37.5% (61.8%) | 63.3% (80.0%) |
| SLy4  | 77.8% (85.8%) | 39.3% (60.7%) | 64.1% (77.6%) |
| FRDM  | 90.9% | 43.1% | 54.4% |

Quantum numbers \((n, \ell, j, m)\) with usual notation) of the last filled orbit, namely \( J = j \) and \( \pi = (-1)^\ell \). In our mean-field approach, this nucleon occupies the first empty level of the self-consistent one-body potential above the lowest-energy levels occupied by the nucleons of the even-even core.

In the FRDM model the single-particle states are obtained by diagonalization of the folded-Yukawa one-body Hamiltonian associated with the GS shape as explained in detail in Ref. [16]. The ground state of the nucleus is approximated by the Slater determinant built from the lowest-energy single-particle states (exhibiting the Kramer’s degeneracy). The spin and parity of an odd nucleus are therefore those of the level occupied by the unpaired nucleon, that is, the highest occupied level for the particle type in odd number [17]. This approximation is implemented for spherical as well as deformed nuclei.

Within the HFBCS model, for computation time reasons, we search for the lowest-energy solution as a function of \( \beta_2 \) defined as in Ref. [13] and calculated exactly for the equivalent spheroid having the same quadrupole moment and mean square radius as the actual nucleus. The variational character of the HFBCS approach ensures that we obtain a minimum with respect to all the other shape degrees of freedom (compatible with the restrained symmetries). In principle we should search for the lowest local minimum in the whole multi-dimensional potential-energy surface, as in the FRDM approach. However this is a formidable task in a Hartree–Fock-like approach and not necessary in many cases. Indeed for several nuclei in various mass regions we have compared HFBCS higher multipole moments from the minimization in the \( \beta_2 \) direction with FRDM ones obtained from a minimization in the full deformation space and found similar nuclear shapes.

Since the potential-energy landscape is affected by the pairing correlations and since the strength of the seniority
force to describe these correlations is not known a priori for a given nucleus, we have to proceed in an iterative way. Starting with the average set of pairing strengths for neutrons and protons, \( g_n = 17 \text{ MeV}/(11 + N) \) and \( g_p = 17 \text{ MeV}/(11 + Z) \) respectively, we determine the local minima of the HFBCS deformation energy as a function of \( \beta_2 \). Then we calculate the pairing strengths from the solution corresponding to the lowest minimum using the pairing model of Möller and Nix [11]. With the new pairing strengths, we determine again the lowest local minimum and repeat this procedure until the \( \beta_2 \) value of the GS minimum converges to within 0.01. The pairing treatment in the FRDM approach is described in detail in Ref. [13].

To solve the Hartree–Fock equations, we diagonalize the one-body Hartree–Fock Hamiltonian in the cylindrical harmonic-oscillator basis. The truncation of the basis and the approximate optimization of its parameters \( b \) and \( q \) are carried out as in Ref. [15]. Although the oscillator parameter \( b \) and the basis size parameter \( N_0 \) scale as \( A^{-1/6} \) and \( A^{1/3} \), respectively, we choose larger values of \( N_0 \) as a function of \( A \), namely values linearly interpolated between \( N_0 = 12 \) for the mass number \( A = 10 \) and \( N_0 = 18 \) for \( A = 260 \), and the optimal value of \( b \) for the spherical shape is taken to be the same for all nuclei, namely \( b_0 = 0.475\text{fm}^{-1} \). We have checked that the GS radii, quadrupole moments, spins and parities of several nuclei across the nuclear chart are not sensitive to the basis size when we retain the above value of \( b_0 \).

We restrict the comparison of the HFBCS results with experimental data to nuclei for which the above models are expected to be valid. We therefore discard the nuclei for which \( 0.01 < \beta_2 < 0.1 \) (interpreted to be soft) and those for which the energy difference \( V_{12} \) between the lowest two minima is less than 2 MeV (to avoid the possible ambiguities associated with shape coexistence).

In Table I we show the corresponding percentage of agreement and the number of successful spin and parity calculations with the SIII, SkM* and SLy4 interactions in the HFBCS model and with the FRDM model, for spherical and deformed nuclei. The same type of information is displayed for each nucleus in the \((N,Z)\) plane, separately for each model approach (three HFBCS and the FRDM calculations) on Figs. 1 to 4.

In deformed nuclei, single-particle levels often lie very close together, which impairs our ability to correctly deduce GS spins and parities. This is particularly true in heavy nuclei since the single-particle level density increases proportionally to \( A \) on average. Such an uncertainty in the determination of the GS spin and parity does not come only from the interactions used, but also from a possible reordering of nuclear levels in odd nuclei with respect to the order deduced from single-particle “bare” spectra caused by the coupling of single-particle degrees of freedom with other (collective) excitation modes. To estimate this uncertainty in the HFBCS calculations we consider not only the lowest-energy quasiparticle but the second lowest quasiparticle excitation as well when it lies at most 1 MeV above the lowest one. The gray (blue online) dots in Figs. 1 to 3 correspond to the nuclei for which the GS spin and parity of the second lowest quasiparticle state agree with the measured values, and the number of such cases is indicated in parenthesis in Table I for each model and deformation category.

FIG. 2: (color online). Same as Fig. 1 with the SkM* interaction.
Calculated GS spin-parity compared to experiment

SLy4
$|\beta_2| \leq 0.01$ or $|\beta_2| \geq 0.10$
$V_{12} \geq 2 \text{ MeV}$

Actinides

FIG. 3: (color online). Same as Fig. 1 with the SLy4 interaction.

FRDM
$|\beta_2| \leq 0.01$ or $|\beta_2| \geq 0.10$
$V_{12} \geq 2 \text{ MeV}$

Actinides

FIG. 4: Same as Fig. 1 within the FRDM model.
In the first line for each model in Table 1 we also indicate in parenthesis the percentage of agreement when considering either of the two lowest quasiparticle excitations.

As for the coupling with the core rotational mode in deformed nuclei, the specific case of single-particle states with $K = 1/2$ has drawn our attention. Depending on the actual value of the decoupling parameter $a$, one may have nuclear GS spins different from 1/2. This happens when $a < -1$ or $a > 4$ and corresponds to about 30% of the cases where $K = 1/2$. In fact we have calculated $a$ only for the lowest-energy quasiparticle when it has $K = 1/2$, so that the actual spin of the second quasiparticle when it has $K = 1/2$ has not been calculated. Therefore the number of gray (blue online) dots in Figs. 1 to 3 is a lower limit. However this does not impair the conclusion drawn about the uncertainty arising from the high single-particle level density in deformed nuclei.

As seen from Table 1 and Figs. 1 to 3 the overall agreement is rather similar for all considered Skyrme forces. One may note, however, that the SIII parameterization is slightly better than the other two. In all four approaches the agreement for the spherical nuclei is much better than for deformed nuclei (partly because of the uncertainty mentioned above for large single-particle level densities). For the spherical nuclei, the FRDM model is more successful than the HFBCS one (90% as compared to 80%, respectively) but with a much smaller set of nuclei, and yields similar results for deformed nuclei, taking only into account the lowest quasiparticle state.

In the mass region $A \leq 100$, including all spherical and deformed nuclei, the agreement is excellent in all HFBCS cases and slightly less good with FRDM (especially for the heaviest nuclei of this mass region). In deformed nuclei in or close to the rare-earth region, FRDM and SIII calculations are equally good and yield slightly better results than the other two Skyrme forces, while in the actinide region the best results are obtained from FRDM and SkM* calculations (with a slight advantage for the former approach).

To conclude this study, we should stress that given the global character of the study (of the order of 400 nuclei involved), the assumptions made to connect calculated single-particle properties with observed spins and parities and the demanding character of such a comparison, the agreement can be deemed significant. This gives thus a rather good level of confidence in the predictive power of these approaches when used in particular contexts. Improvements of this comparative study should include a more sophisticated treatment of the coupling of single-particle and collective degrees of freedom.

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