Skyrme mean-field studies of nuclei far from the stability line

P.-H. Heenen,*1 P. Bonche,*2 S. Ćwiok*3, W. Nazarewicz*4−*6 and A. Valor*1

*1 Physique Nucléaire Théorique, University of Brussels, Belgium
*2 SPHT, CEA, Saclay, France.
*3 Institute of Physics, Warsaw University of Technology, Poland
*4 Department of Physics, University of Tennessee, Knoxville, USA
*5 Physics Division, Oak Ridge National Laboratory, USA
*6 Institute of Theoretical Physics, University of Warsaw, Poland

Two applications of mean-field calculations based on 3D coordinate-space techniques are presented. The first concerns the structure of odd-N superheavy elements that have been recently observed experimentally and shows the ability of the method to describe, in a self-consistent way, very heavy odd-mass nuclei. Our results are consistent with the experimental data. The second application concerns the introduction of correlations beyond a mean-field approach by means of projection techniques and configuration mixing. Results for Mg isotopes demonstrate that the restoration of rotational symmetry plays a crucial role in the description of $^{32}$Mg.

Introduction

Mean-field calculations on a 3-dimensional mesh were introduced in nuclear physics in the late 1970s in the studies of nuclear collisions within the time-dependent Hartree-Fock method\(^1\). In these early applications, schematic nuclear interactions were used, without spin-orbit and Coulomb terms, and applications were limited to collisions between light nuclei. The same technique has later been applied in a systematic study of the spectroscopic properties of Zr and neighboring isotopes\(^2\). New developments have then permitted the use of effective interactions of the Skyrme type, including Coulomb and spin-orbit terms, and pairing correlations were considered the BCS approximation with a seniority force. There are several advantages of the coordinate-space technique which make it very attractive. It allows one to describe very general intrinsic deformation with a good numerical accuracy. It also provides a very flexible computation scheme, suitable for generalizations (e.g., introduction of correlations beyond the mean-field theory). The main developments of the method performed after the completion of the Zr study were the introduction of a cranking constraint to describe rotating nuclei\(^3\), the introduction of the configuration mixing using the generator coordinate method\(^4\), the particle-number projected HF+BCS calculations\(^5\), and improvements in the treatment of the pairing correlations by the use of the HFB method\(^6\) with density-dependent zero-range interactions\(^7\). Let us also mention a theoretical study of the properties of coordinate-space calculations\(^8\) which introduced powerful ways to interpolate wave functions discretized on a 3D mesh.

In this note, we shall first present a very representative application of the method to odd-N superheavy elements\(^9\) (SHE). We shall then describe new developments\(^10\) related to the restoration of the rotational and particle number symmetries; these improvements are expected to be extremely useful in future studies of medium-mass nuclei far from stability.

Structure of Odd-$N$ Superheavy Elements

There is no consensus among theorists with regard to the center of the shell stability in the region of spherical SHE. For the neutrons, most calculations predict a magic gap at $N=184$. However, because of different treatments of the large Coulomb potential and spin-orbit interaction, various models yield different predictions for the position of the magic proton gap (cf. discussion in Ref.\(^11\)). In this context, the synthesis of the $N=175$ isotones reported by the Dubna/Livermore (DL) collaboration ($Z=114$)\(^12\) and the Berkeley/Oregon (BO) team ($Z=118$)\(^13\) is particularly important. Due to the large neutron number of the compound nucleus, the observed $\alpha$ chains do not terminate at some known systems. Consequently, until the charge-mass identification is made, one can use theoretical arguments to support/disprove the experimental assignment.

We have performed a large-scale self-consistent study of properties of even-even, $A$-odd, and odd-odd heaviest nuclei. In our work, we have used the Hartree-Fock-Bogoliubov (HFB) method with a Skyrme interaction in the particle-hole (ph) channel and a delta force in the pairing channel. The details of the calculations closely
Table 1. Predicted structure of the lowest one-quasiparticle excitations in the $^{289}114 \alpha$-decay chain. Each excitation is characterized by the Nilsson quantum numbers of the odd neutron, excitation energy, and quadrupole deformation. The number in parentheses indicates the $Q_\alpha$ value for the ground-state to ground-state transition.

| Nucleus | Orbital | Energy (MeV) | $\beta_2$ |
|---------|---------|--------------|-----------|
| $^{289}114$ | $[707]_{15}^{-}$ | 0.12 | 0.04 |
| (9.64) | $[611]_{4}^{+}$ | 0.52 | 0.15 |
| $^{285}112$ | $[611]_{4}^{+}$ | 0.60 | 0.15 |
| (8.88) | $[707]_{15}^{-}$ | 0.62 | 0.14 |
| | $[600]_{4}^{+}$ | 0.65 | 0.14 |
| | $[604]_{4}^{+}$ | 0.72 | 0.14 |
| $^{281}110$ | $[604]_{3}^{+}$ | 0.07 | 0.14 |
| (9.32) | $[600]_{3}^{+}$ | 0.12 | 0.13 |
| | $[611]_{4}^{+}$ | 0.59 | 0.17 |
| | $[613]_{3}^{+}$ | 0.65 | 0.17 |
| $^{277}108$ | $[611]_{3}^{+}$ | 0.04 | 0.20 |
| | $[604]_{3}^{+}$ | 0.31 | 0.20 |
| | $[710]_{25}^{-}$ | 0.36 | 0.21 |

Table 2. Same as in Table 1, except for the $^{293}118 \alpha$-decay chain.

| Nucleus | Orbital | Energy (MeV) | $\beta_2$ |
|---------|---------|--------------|-----------|
| $^{293}118$ | $[707]_{15}^{-}$ | 0.12 | 0.04 |
| (11.59) | $[611]_{4}^{+}$ | 0.16 | 0.10 |
| | $[602]_{4}^{+}$ | 0.84 | 0.12 |
| | $[604]_{4}^{+}$ | 0.98 | 0.10 |
| $^{289}116$ | $[611]_{4}^{+}$ | 0.12 | 0.04 |
| (10.18) | $[606]_{3}^{+}$ | 0.62 | 0.14 |
| | $[611]_{4}^{+}$ | 0.66 | 0.14 |
| | $[604]_{4}^{+}$ | 0.69 | 0.14 |
| | $[707]_{15}^{-}$ | 0.72 | 0.14 |
| $^{285}114$ | $[606]_{1}^{+}$ | 0.04 | 0.14 |
| (10.60) | $[611]_{1}^{+}$ | 0.15 | 0.14 |
| | $[613]_{2}^{+}$ | 0.16 | 0.14 |
| $^{281}112$ | $[611]_{2}^{+}$ | 0.07 | 0.14 |
| (10.85) | $[604]_{2}^{+}$ | 0.37 | 0.19 |
| | $[613]_{2}^{+}$ | 0.41 | 0.19 |

The HFB equations have been solved in the coordinate space according to the method of Ref. 7. In the ph channel, the Skyrme effective interaction SLy4 has been used. This parameterization has, in particular, been adjusted to reproduce long isotopic sequences; hence, one can expect it to have good isospin properties. The pairing strengths of the interaction have then been adjusted to reproduce the average proton and neutron pairing gaps in even-even nuclei around $^{254}$Fm. The properties of one-quasiparticle states were calculated by means of the self-consistent blocking.

The calculated one-quasiparticle structures and the g.s.-to-g.s. values of $Q_\alpha$ in the $^{289}114$ and $^{293}118 \alpha$-decay chains are shown in Tables 1 and 2, respectively.

According to our calculations, the g.s.-to-g.s. $\alpha$ decays of $^{289}114$ and $^{293}118$ are structurally forbidden since the g.s. properties of parent and daughter nuclei differ dramatically. The allowed transitions to the excited $[707]_{15}^{-}$ level in $^{285}112$ and $^{289}116$ correspond to $Q_\alpha=9.0$ MeV and $Q_\alpha=10.9$ MeV, respectively, and are considerably lower than the experimental values (DL: 9.9 MeV; BO: 12.6 MeV) Consequently, the most probable candidates for the first $\alpha$ transitions are the 10.2 MeV ($^{289}114$) and 11.8 MeV ($^{293}118$) lines associated with the allowed $[611]_{4}^{+}$ to $[611]_{4}^{+}$ decays. By the same token, the $[611]_{2}^{+}$ g.s. of $N=173$ isotones is expected to decay to the excited $[611]_{2}^{+}$ level in the $N=171$ daughters. For $^{285}112$, the corresponding $Q_\alpha$ energy, 8.76 MeV, is very close to the experimental energy of the second $\alpha$ transition, 8.84 MeV, reported by the DL group. For the $^{289}116$ decay we obtain $Q_\alpha=10.14$ MeV; i.e., we underestimate the energy of the second $\alpha$ particle (11.8 MeV) from the BO experiment. This is the worst deviation from experiment obtained in our calculations.

The $[611]_{4}^{+}$ level is also expected to be the ground state of the $N=169$ isotones, and our prediction for the allowed $[61]_{4}^{+}$ to $[61]_{4}^{+}$ decays is 9.4 MeV for $^{281}110$ (DL: 9.0 MeV) and 10.6 MeV for $^{285}114$ (BO: 11.5 MeV).

For the $\alpha$ transitions in the $^{281}112$→⋯→$^{265}104$ chain, allowing the positive-parity Nilsson orbitals with very similar quantum numbers, we obtain the following values of $Q_\alpha$: 10.7 MeV (BO: 10.8 MeV), 11.1 MeV (BO: 10.3 MeV), 9.9 MeV (BO: 9.9 MeV), 8.0-8.5 MeV (BO: 8.9 MeV). An alternative route is possible that involves $\alpha$ transitions between $j_{15/2}$ orbitals. Here, for the last two $Q_\alpha$ values we obtain 9.8 MeV and 8.7 MeV. In both cases we obtain good agreement with BO data.

The calculated equilibrium deformations of one-quasiparticle states in $N=175$ isotones are rather small ($\beta_2 \approx 0.11$), and they increase along the $\alpha$-decay chain. This trend reflects the influence of the $N=184$ magic neutron gap for the heaviest systems and the deformed $N=162$ gap for the lightest nuclei in the chain. As far as $Q_\alpha$ values are concerned, our calculations are consistent with the recent experimental findings.
Correlations beyond mean field in Mg isotopes

The cranking method is widely used in nuclear spectroscopy to describe high-spin states. Applications based on effective nuclear interactions have been particularly successful in the description of superdeformed rotational bands in several regions of the mass table. In the cranking method, a rotational band is generated by the rotation of a deformed intrinsic state. Since cranking states are not eigenstates of the angular momentum, this causes some problems in determining, e.g., transition rates in nuclei which are not very well deformed.

Another limitation of the cranking model appears in nuclei which are soft with respect to the variation of a collective variable. In this case, one expects the interference of the zero-point vibrational mode with the rotational motion which leads to variations in the nuclear structure.

In ref \(^5\), we have presented a method to restore the particle number symmetry within the HF+BCS theory that allows us to perform a configuration mixing of projected wave functions in the direction of selected collective variables. The method presented in this section generalizes it by the inclusion of a restoration of the rotational symmetry. It enables us to describe details of collective spectra and transition rates.

The starting point of the method are wave functions \(|\Phi_\alpha\rangle\) generated by mean-field calculations with a constraint on a collective coordinate \(\alpha\). Wave functions with good angular momentum and particle numbers,

\[
|\Phi, JM\alpha\rangle = \frac{1}{N_x} \sum_K g_K \hat{P}_M^J \hat{P}_N^Z |\Phi_\alpha\rangle,
\]  

are obtained by means of the projection operators \(\hat{P}\). In Eq. (1), \(N_x\) is a normalization factor, depending on \(x = J, M, N, Z, \alpha\).

Using the projected state \(|\Phi, JM\alpha\rangle\) as a generating function, configuration mixing along the collective variable \(\alpha\) is performed for each angular momentum:

\[
|\Psi, JM\rangle = \sum_\alpha f^{JM}_\alpha |\Phi, JM\alpha\rangle.
\]

The weight functions \(f^{JM}_\alpha\) are found by requiring that the expectation value of the energy,

\[
E^{JM} = \frac{\langle \Psi, JM | \hat{H} | \Psi, JM \rangle}{\langle \Psi, JM | \Psi, JM \rangle},
\]

is stationary with respect to an arbitrary variation \(\delta f^{JM}_\alpha\).

This prescription leads to the discretized Hill-Wheeler equation

\[
\sum_\alpha (H^{JM}_{\alpha,\alpha'} - E^{JM}_k I^{JM}_{\alpha,\alpha'}) f^{JM}_{\alpha,\alpha'} = 0,
\]

in which the Hamiltonian kernel \(H^{JM}_{\alpha,\alpha'}\) and the overlap kernel \(I^{JM}_{\alpha,\alpha'}\) are defined as

\[
H^{JM}_{\alpha,\alpha'} = \langle \Phi, JM|\hat{H}|\Phi, JM'\rangle, \quad I^{JM}_{\alpha,\alpha'} = \langle \Phi, JM|\Phi, JM'\rangle.
\]

The kernels \(I\) are obtained by integrating the matrix elements between rotated wave functions over three Euler angles and two gauge angles. Besides these kernels, one can determine transition probabilities between different eigenstates of the Hill-Wheeler equation. This requires the calculation of matrix elements of electromagnetic operators.

Currently, in order to save computing time and to test the method, certain symmetry restrictions have been imposed on the mean-field wave functions. Namely, they have been assumed to be axially symmetric and time-reversal invariant. In this way, the integration over the Euler angles is limited to a single angle. Pairing correlations are treated in the BCS approximation.

In the following examples, a Skyrme force is used in the particle-hole channel and a density-dependent zero-range interaction in the pairing channel. As in ref \(^5\), in the calculation of non-diagonal matrix elements, the density dependence of the Skyrme interaction is generalized to a dependence on the mixed density.

Application to \(^{24}\)Mg

The results shown in this section have been obtained using the HF+BCS wave functions generated with an axial quadrupole constraint. The Lipkin-Nogami prescription has been used to improve the treatment of pairing correlations. The variation of the energy as a function of prolate and oblate deformations is plotted in Fig. 1 for the Sly4 Skyrme interaction and a surface pairing interaction having strength \(G=1000\text{MeV fm}^3\) for both neutrons and protons. In addition to the prolate absolute minimum, the mean-field curve presents a shoulder at an oblate deformation around 50 fm\(^2\). The triple projection creates an oblate minimum at the position of the shoulder for \(J\) up to 6\(^+\). For greater values of \(J\), the weights of the intrinsic wave functions for deformations below –200 fm\(^2\) are very small. Consequently, the projected energy curves do not exhibit any oblate minima.

For each value of the angular momentum, we have performed a configuration-mixing calculation including quadrupole moments between –350fm\(^2\) and 450 fm\(^2\). This corresponds to intrinsic configurations excited by about 30 MeV with
respect to the prolate minimum. The spectrum that is generated in this way (represented by bars) is plotted at the quadrupole moment corresponding to the largest component of the collective wave function. The value of this quadrupole moment is very close to the minimum of the projected energy curve. Moreover, the energy of this minimum is only slightly modified by the configuration mixing. The largest gain, \( \sim 800 \text{ keV} \), is obtained for the \( 0^+ \) state, but it is reduced at higher spins. Several excited states are found at low energy for each spin value. Except for the second \( 0^+ \) and \( 10^+ \), the wave functions of yrare states are peaked around the oblate secondary minimum.

In the same figure, theoretical transition probabilities along the yrast line are compared with the data. In the GCM calculation, the minima of projected energy curves have been used. The \( B(E2; 2^+_1 \rightarrow 0^+_1) \) rate calculated between the minima of the two curves is very close to the experimental value. The configuration mixing causes a spreading of the collective wave function on the quadrupole moment and decreases the value of the \( B(E2) \) rate. Since for spins greater than zero wave functions do not have low quadrupole-moment components, the configuration mixing does not affect significantly the transition probabilities. Here, the agreement between calculations and experiment is excellent. One has to note, however, that the inclusion of triaxiality is expected to modify these predictions to some extent.

**Application to \( ^{32}\text{Mg} \)**

Although \( ^{32}\text{Mg} \) corresponds to the \( N=20 \) shell closure, there is some experimental evidence that it is deformed in its ground state. The excitation energy of its first \( 2^+ \) state is only around 900 keV, i.e., significantly lower than in lighter Mg isotopes. Also the \( 4^+ \) state, but it is reduced at higher spins. Several excited states are found at low energy for each spin value. Except for the second \( 0^+ \) and \( 10^+ \), the wave functions of yrare states are peaked around the oblate secondary minimum.

Figure 2 shows the calculated energy curves for \( ^{32}\text{Mg} \). The ground state calculated in the HF+BCS approximation is spherical (see discussion in ref.\(^{15}\)). However, unlike in the \( ^{24}\text{Mg} \) case, the restoration of broken symmetries modifies the topology of the energy curve in a more dramatic way. Namely, the resulting \( 0^+ \) ground state corresponds to the projection of a deformed intrinsic state with a quadrupole moment of 100 fm\(^2\). The minima for the higher-\( J \) values can be associated with even larger deformations. The configuration mixing leads to small energy gains. The collective \( 0^+ \) wave function is spread over a large range of quadrupole moments between \(-200\text{ fm}^2\) and \(200\text{ fm}^2\), while for other \( J \)-values the weights of the HF+BCS wave functions have well-pronounced maxima around \(200\text{ fm}^2\).

The calculated spectrum and transition probabilities are compared to the experimental data in Fig. 2. It is seen that our calculations do not reproduce the pronounced collectivity of \( ^{32}\text{Mg} \). Compared to the data, the energy of the \( 2^+ \) is too high and the \( B(E2) \) value is too low. It should be noted, however, that the delicate balance between the spherical minimum and the deformed intruder configuration in this nucleus is sensitive to the effective interaction used\(^{15}\).

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Fig. 1. Symmetry-projected results for the nucleus $^{24}\text{Mg}$. (a) Energies as a function of the axial quadrupole moment. Solid line with stars: HF+BCS+LN results; the curves displaying filled circles, filled boxes, filled diamonds, circles, boxes, and diamonds correspond, respectively, to projected energies in the $J=0^+$, $2^+$, $4^+$, $6^+$, $8^+$, $10^+$ states. The horizontal bars are the projected energies of the collective intrinsic states. (b) Excitation energies and transition probabilities (numbers in e²fm⁴) between: intrinsic states minimizing each projected energy curve (left), yrast collective states (right), and experimental levels (center).
Fig. 2. Same as in Fig. 1, except for $^{32}$Mg.