COLLECTIVE EXCITATIONS OF TRANSACTINIDE NUCLEI IN A
SELF-CONSISTENT MEAN FIELD THEORY

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Received (October 31, 2007)
Revised (revised date)

We applied the ATDHFB approach for study of properties of collective quadrupole states
in several transactinide nuclei: $^{238}\text{U}$, $^{240}\text{Pu}$, $^{242}\text{Pu}$, $^{246}\text{Cm}$, $^{248}\text{Cm}$, $^{250}\text{Cf}$ and $^{252}\text{Cf}$. Calculated energies and $\text{B(E2)}$ transition probabilities are in a reasonable agreement
with experimental data. We present also results concerning superdeformed collective
states in the second minimum of potential energy of the $^{240}\text{Pu}$ nucleus.

1. Introduction

Fission properties of heavy and superheavy nuclei have been recently a subject
of intensive studies within the frame of a self-consistent mean field theory. Most
papers treated height of fission barriers but some results on half-lives of
superheavy nuclei have also been published. The standard method of calculating
the half-lives is the WKB(J) approach requiring knowledge of the potential and
mass parameter(s), which are usually obtained from the Adiabatic Time Depen-
dent Hartree-Fock-Bogolyubov (ATDHFB) or the Generating Coordinate Method
(GCM) theory. These general theories can provide a frame for a description of other
collective phenomena, e.g. quadrupole rotational-vibrational excitations. However
such applications of ATDHFB or GCM in the region of transactinides are rather
scarce. On the other hand collective levels and $\text{E2}$ transition probabilities of lighter
transactinides ($\text{U,Pu,Cm}$) are well known experimentally. Moreover thanks to re-
cent advances in experimental techniques the region of heavier nuclei accessible for
measurements is growing rapidly. In this paper we present several results of applica-
tion of the ATDHFB theory with the Skyrme interaction for describing quadrupole
collective properties of $^{238}\text{U}$, $^{240}\text{Pu}$, $^{242}\text{Pu}$, $^{246}\text{Cm}$, $^{248}\text{Cm}$, $^{250}\text{Cf}$ and $^{252}\text{Cf}$ nuclei,
for which there is an abundant experimental data. The main part of the paper is
devoted to normally deformed states, i.e., built around the first minimum of the
potential energy but Subsection contains also results of calculation of superde-
formed (connected with the second minimum of the potential) states in the $^{242}\text{Pu}$
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2. Theory

The main tool used in microscopic theory of full five-dimensional quadrupole collective dynamics is the ATDHFB theory, which leads to the generalized Bohr Hamiltonian when appropriate collective variables are chosen. The collective Hamiltonian contains potential energy and mass parameters (including moments of inertia) calculated solely from a microscopic input, i.e., nucleon-nucleon interaction. Details of the method we use and results obtained for lighter nuclei can be found in. 7, 8 Below we recall only some of main points.

Collective quadrupole variables $\beta$, $\gamma$ are defined by components of the second rank tensor of a nuclear mass distribution:

\[
\begin{align*}
\beta \cos \gamma &= q_0 \sqrt{\frac{\pi}{5}/A} \langle r^2 \rangle, \quad r_0 = 1.2 \text{fm} \\
\beta \sin \gamma &= q_2 \sqrt{\frac{3\pi}{5}/A} \langle r^2 \rangle \\
q_0 &= \langle Q_0 \rangle = \langle \sum_i 3z_i^2 - r_i^2 \rangle \\
q_2 &= \langle Q_2 \rangle = \langle \sum_i x_i^2 - y_i^2 \rangle.
\end{align*}
\]

Hence in the axial case $\beta$ for a given nucleus is strictly proportional to the mass quadrupole moment. The self-consistent nuclear mean field is obtained from HF+BCS calculations with a double constraint:

\[
\delta(H - \lambda_0 Q_0 - \lambda_2 Q_2) = 0.
\]

Then the ATDHFB theory allow to calculate mass parameters and collective potential energy that enter the Bohr Hamiltonian. Its eigenvalues are interpreted as collective excitation energies and its eigenfunctions can be used, among others, to obtain E2 transition probabilities.

2.1. Details of calculations

We have chosen as a microscopic interaction the SkM* version of Skyrme forces, proposed already long time ago 9 but still regarded as a good choice especially in the case of barrier heights and other fission properties. 2, 4, 6 We have performed also calculations with the SIII Skyrme interaction which previously gave good results for lighter nuclei 7 and a few tests with the more recent SLy4 forces. In the particle-particle channel we have taken the simplest form of the pairing interaction i.e. of seniority type (constant $G$). Strength of the pairing was fixed by comparing values of the 5-point formula pairing gap with minimal quasiparticle energies at points corresponding to a minimum of the potential in U and Pu nuclei. Final results for the strength are $G_{n,p} = g_{n,p}/(11 + N(Z))$, $g_n = 15.1$ MeV, $g_p = 14.9$ MeV. As we checked in some test cases the results from a state dependent ($\delta$) pairing interaction are almost the same as from the constant $G$ force, provided the strength of the interaction is fixed using the same method.

The calculations were made for 220 points in the sextant ($0 \leq \gamma \leq 60^\circ$, $0 \leq \beta \leq 1$) of the deformation plane. These point form a regular grid with the distance of 0.05 and 6° between them. The maximal value of $\beta$ (i.e. $\beta = 1$) corresponds for the
considered nuclei to a quadrupole moment around 100 b. For the lowest normally deformed collective states only the region $\beta \lesssim 0.6$ is important but for studying the second minimum one must expand the range of $\beta$ considerably.

It must be stressed that we exclude the octupole deformation which is essential for fission processes, but for the considered nuclei it becomes important only for larger deformations than those studied by us. As we discussed previously in [10,11,12], pairing vibrations and so called Thouless-Valatin corrections can have a noticeable influence on the mass parameters. In the present work we took a simplified approach introducing an average factor 1.3 by which we multiply values of the mass parameters obtained from the ATDHFB formulas.

For each nuclei we calculate seven functions (the potential energy and six mass parameters, including moments of inertia). In Fig. 1, we show only a small sample, namely the potential energy $V$ and the mass parameter $B_{\beta\beta}$ for the $^{242}$Pu nucleus.

![Fig. 1. Collective potential energy $V$ (left panel) and the mass parameter $B_{\beta\beta}$ (right panel) for the $^{242}$Pu nuclie.](image)

3. Results

3.1. Energy levels

In Fig. 2, we show a calculated energy of the first $2^+_{g.s.}$ level and of bandheads of $\beta$ and $\gamma$ bands and we compare them with experimental data [13]. Please note that the energies (theoretical and experimental) of the $2^+_{g.s.}$ level are multiplied by 5 to make the figure more readable. Keeping in mind the starting point of calculations which was the nucleon-nucleon effective interaction and the fact that we did not fit any parameter to analyzed data, the results shown in Fig. 2 are quite good, even despite too large energies of the theoretical $\beta$ and $\gamma$ bandheads.

Below we present also analogous results for the SIII Skyrme interaction (Fig. 3).
As it can be seen the $\beta$ and $\gamma$ bandheads are now on average closer to experimental values, but their behavior with an increasing mass number does not follow the experimental one. Detailed inspection of calculated potential energy and mass pa-

Fig. 3. See caption to Fig. 2, theoretical levels are obtained using the SIII Skyrme interaction.

rameters shows that differences between the results of the SkM* and SIII variant of Skyrme interaction stem mainly from different behavior of the potential in the region of small deformations. It can be readily seen in Fig. 4 where we plot the
potential energy for axial shapes of the $^{242}$Pu nucleus obtained using the SkM*, SIII and SLy4 forces. This figure shows also that dependence of $V$ on deformation for the SkM* and SLy4 forces is very similar.

Fig. 4. Comparison of the potential energy calculated for axial shapes of the $^{242}$Pu nucleus using various Skyrme interaction. In this figure negative values of $\beta$ correspond to an oblate shape.

Let us mention another remarkable point. In many papers the energy of the first $2^+$ level is estimated from the formula $E_{2,\text{rot}} = 2(2 + 1)/2J$, where $J$ is the moment of inertia calculated in the minimum of the potential, in other words assuming a perfect rotor behavior. Within the frame of our approach we can compare the value obtained in such a way with the respective eigenvalue of the Bohr Hamiltonian $E_{2,\text{Bohr}}$. It appears that $E_{2,\text{Bohr}}$ is greater typically by 16–20 keV than $E_{2,\text{rot}}$. This correction comes from vibrational degrees of freedom and is very small if compared with the energy of, loosely speaking, $\beta$ and $\gamma$ phonons but is quite large in relation to $E_{2,\text{exp}}$.

3.2. $E2$ electromagnetic transitions

In this subsection we compare theoretical $B(E2)$ transition probabilities with the experimental ones, taken from\[13\] Fig. 5 shows transitions $2_{gs} \rightarrow 0_{gs}$ in the considered nuclei while Fig. 6 contains results concerning transitions within the ground state band in the $^{248}$Cm nucleus. Moreover in Table 1 we present some inter-band transitions in the $^{250}$Cf nucleus.

| $2^+$ (γ band) → g.s. | Exp | SkM* | S III |
|-----------------------|-----|------|-------|
| $2^+$                  | 0.21 ± 0.02 | 0.87 | 0.49  |
| $0^+$                  | 3.7 ± 0.4   | 10.32| 8.16  |
|                       | 2.3 ± 0.3   | 6.26 | 4.73  |

The conclusion is that theoretical results follow experiment very closely. We
Fig. 5. $B(E2)$ probabilities for transition $2_{gs} \rightarrow 0_{gs}$. Experimental data taken from [13].

Fig. 6. $B(E2)$ transition probabilities within the ground state band in the $^{248}$Cm nucleus. $J_i$ denotes spin of an initial level.

recall again that we do not use here any additional parameters (effective charge etc.). And again the SIII interaction performs slightly better than SkM*.

3.3. Superdeformed collective states

Theory presented in the previous sections gives also possibility to study superdeformed collective states i.e. built in the vicinity of the second minimum of the potential energy. It needs however a large extension of the basis used to solve the eigenproblem of the Bohr Hamiltonian. We presented such calculations in the approach with the phenomenological Nilsson potential in Ref. [14], see also papers by Libert et al. using Gogny forces [12]. In the present paper we show results for the $^{242}$Pu nucleus, for which there are many experimental data [15], see also review in Ref. [5]. Moreover in this nucleus an outer barrier is sufficiently high (see also Fig. 4), so as we do not need to worry about e.g. coupling with the continuum.

Fig. 7 shows the probability distribution for the ground state and the lowest $J = 0$ state that can be unambiguously identified as a superdeformed one. More precisely we plotted here the product $|\Psi|^2 \sqrt{\det g}$, where $g$ is the metric tensor in the collective space.

Table 2 contains more detailed information on the calculated properties of the lowest normally and super deformed states in the $^{240}$Pu nucleus. We show here also the average values $\langle \beta \rangle$ and $\langle \gamma \rangle$. 
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Fig. 7. Probability distribution $|\Psi|^2 \det g$ for the lowest $0^+$ normal (i.e. ground) and superdeformed state.

Table 2. Lowest normal and superdeformed states $J = 0$ and 2 in $^{240}$Pu (in MeV).

| J  | #  | $\langle \beta \rangle$ | $\langle \gamma \rangle$ | $E_{\text{th}}$ | $E_{\text{exp}}$ | $(E - E_{0,\text{SD}})_{\text{th}}$ | $(E - E_{0,\text{SD}})_{\text{exp}}$ |
|----|----|----------------|----------------|-----------|-----------|----------------|----------------|
| ND | 0  | 0.299          | 8.09           |           |           |               |               |
|    | 2  | 0.299          | 8.07           | 0.046     | 0.043     |               |               |
|    | 0  | 0.315          | 10.54          | 1.420     | 0.860     |               |               |
|    | 2  | 0.315          | 10.50          | 1.470     | 0.900     |               |               |
|    | 2  | 0.314          | 13.07          | 1.547     | 1.137     |               |               |
| SD | 0  | 0.829          | 2.94           | 4.321     | 2.55      |               |               |
|    | 2  | 0.829          | 2.94           | 4.342     | 0.021     |               |               |
|    | 0  | 0.836          | 3.52           | 5.472     | 1.151     |               | 0.77           |
|    | 2  | 0.835          | 3.53           | 5.494     | 1.173     |               |               |

$^a$ # denotes the number of a state for a given spin.

Obtained qualitative agreement with experiment looks rather encouraging. Moreover, one must remember that we have not included in our calculation the so called rotational correction often discussed in papers on fission barriers. Its magnitude increases with a deformation and in consequence superdeformed states can be lowered by 0.8-0.9 MeV. However in our opinion a consistent introduction of this correction into our formalism (keeping in view also allowed triaxial shapes of a nucleus) needs more careful treatment.

4. Conclusions

The ATDHFB approach offers a considerable extension of the area of applicability of the self-consistent mean field theory, namely on low energy collective states, for which there is often rich spectroscopic data. Our study shows that starting with standard Skyrme interactions one can obtain reasonable description of energies and $B(E2)$'s also for very heavy nuclei. However some problems still remain open, e.g. questions concerning the Thouless-Valatin corrections, pairing vibrations, rotational and other so called zero point energy corrections.
Acknowledgments

Present work was partially supported by the Academy of Finland and Jyväskylä University within the FiDiPro programme.

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