Multidimensionally constrained relativistic mean field model and applications in actinide and transfermium nuclei

Bing-Nan Lu, Jie Zhao, En-Guang Zhao and Shan-Gui Zhou

1 State Key Laboratory of Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, People’s Republic of China
2 Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator, Lanzhou 730000, People’s Republic of China

E-mail: sgzhou@itp.ac.cn

Received 15 November 2013
Accepted for publication 16 December 2013
Published 29 April 2014

Abstract
We present some results of potential energy surfaces of actinide and transfermium nuclei from multidimensionally constrained relativistic mean field (MDC-RMF) models. Recently we developed multidimensionally constrained covariant density functional theories (MDC-CDFT), in which all shape degrees of freedom $\beta_{\lambda \mu}$ with even $\mu$ are allowed, and the functional can be one of the following four forms: the meson exchange or point-coupling nucleon interactions combined with the nonlinear or density-dependent couplings. In MDC-RMF models, the pairing correlations are treated with the BCS method. With MDC-RMF models, the potential energy surfaces of even–even actinide nuclei were investigated and the effect of triaxiality on the fission barriers in these nuclei was discussed. The nonaxial reflection-asymmetric $\beta_{32}$ shape in some transfermium nuclei with $N = 150$, namely $^{246}$Cm, $^{248}$Cf, $^{250}$Fm and $^{252}$No, were also studied.

Keywords: covariant density functional theory, potential energy surface, actinide nuclei, transfermium nuclei

(Some figures may appear in colour only in the online journal)

1. Introduction

The occurrence of spontaneous symmetry breaking in atomic nuclei leads to various nuclear shapes, which can usually be described by the parametrization of the nuclear surface or the nucleon density distribution [1, 2]. In mean-field calculations, the following parametrization

$$\beta_{\lambda \mu} = \frac{4\pi}{3AR} \langle Q_{\lambda \mu} \rangle,$$

(1)

is usually used, where $Q_{\lambda \mu}$ are the mass multipole operators. In figure 1, a schematic is given for some typical nuclear shapes. The majority of observed nuclear shapes are of spheroidal form, which is usually described by $\beta_{20}$. Higher-order deformations with $\lambda > 2$ such as $\beta_{50}$ also appear in certain atomic mass regions [3]. In addition, nonaxial shapes in atomic nuclei, in particular, the nonaxial-quadrupole (triaxial) deformation $\beta_{22}$, have been studied both experimentally and theoretically [4–6]. The influence of the nonaxial octupole $\beta_{32}$ deformation on the low-lying spectra has also been investigated [7–16].

In nuclear fission study, various shape degrees of freedom play important and different roles in the occurrence and in determining the heights of the inner and outer barriers in actinide nuclei (in these nuclei, double-humped fission barriers usually appear). For example, the inner fission barrier is
usually lowered when the triaxial deformation is allowed, while for the outer barrier the reflection asymmetric (RA) shape is favored [18–24].

In order to give a microscopic and self-consistent description of the potential energy surface (PES) with more shape degrees of freedom included, multidimensionally constrained covariant density functional theories were developed recently [25, 26]. In these theories, all shape degrees of freedom $\lambda \mu$ with even $\mu$ are allowed. In this contribution, we present two recent applications of these theories: the PESs of actinide nuclei and the nonaxial reflection-asymmetric $32^\beta$ shape in some transfermium nuclei. In section 2, the formalism of our multidimensionally constrained covariant density functional theories will be given briefly. The results and discussions are presented in section 3. Finally, we give a summary in section 4.

2. Formalism

The details of the formalism for covariant density functional theories can be found in [27–32]. The CDFT functional in our multidimensionally constrained calculations can be one of the following four forms: the meson exchange or point-coupling nucleon interactions combined with the nonlinear or density-dependent couplings [25, 26, 33, 34]. Here we show briefly the one corresponding to the nonlinear point coupling (NL-PC) interactions. The starting point of the relativistic NL-PC density functional is the following Lagrangian:

$$\mathcal{L}_{\text{lin}} = \frac{1}{2} a_5 \rho_S^2 + \frac{1}{2} a_V \rho_V^2 + \frac{1}{2} \alpha_{TS} \rho_{TS}^2 + \frac{1}{2} \alpha_{TV} \rho_{TV}^2,$$

$$\mathcal{L}_{al} = \frac{1}{3} \rho_S^3 + \frac{1}{4} \rho_V^4 + \frac{1}{4} \rho_{TS}^4,$$

$$\mathcal{L}_{\text{der}} = \frac{1}{2} \delta_S \left[ \partial \rho_S \right]^2 + \frac{1}{2} \delta_V \left[ \partial \rho_V \right]^2 + \frac{1}{2} \delta_{TS} \left[ \partial \rho_{TS} \right]^2 + \frac{1}{2} \delta_{TV} \left[ \partial \rho_{TV} \right]^2,$$

$$\mathcal{L}_{\text{Cou}} = \frac{1}{4} F^\mu F_{\mu} + e \left( 1 - \frac{\tau_5}{2} \right) A_\mu \rho_V,$$  

are the linear coupling, nonlinear coupling, derivative coupling and Coulomb part, respectively. $M$ is the nucleon mass, $\alpha_S, \alpha_V, \alpha_{TS}, \alpha_{TV}, \gamma_S, \gamma_V, \delta_S, \delta_V, \delta_{TS}$ and $\delta_{TV}$ are coupling constants for different channels and $e$ is the electric charge. $\rho_S, \rho_V$ and $\rho_{TS}$ are the isoscalar density, isovector density, time-like components of isoscalar current, and time-like components of isovector current, respectively. The densities and currents are defined as

$$\rho_S = \bar{\psi} \psi, \quad \rho_V = \bar{\psi} \gamma^\mu \psi, \quad \rho_{TS} = \bar{\psi} \gamma^\mu \tau_5 \psi, \quad \rho_{TV} = \bar{\psi} \gamma^\mu \tau_3 \psi.$$  

Starting from the above Lagrangian, using the Slater determinants as trial wave functions and neglecting the Fock term as well as the contributions to the densities and currents from the negative energy levels, one can derive the equations of motion for the nucleons,

$$\hat{h} \psi = (\alpha \cdot \vec{p} + \beta (M + S(\vec{r})) + V(\vec{r})) \psi = \epsilon \psi,$$  

where

$$S = \alpha_S \rho_S + \beta_S \rho_S^2 + \gamma_S \rho_S^3 + \delta_S \Delta \rho_S$$

$$+ \left[ \alpha_{TS} \rho_{TS} + \delta_{TS} \Delta \rho_{TS} \right] \tau_5,$$  

are the potential $V(r)$ and $S(r)$ are calculated as

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$\beta_{\lambda \mu}$ & $\beta_{20}$ & $\beta_{20}$ & $\beta_{40}$ \\
\hline
$= 0$ & $> 0$ & $< 0$ & $\neq 0$ \\
\hline
$\neq 0$ & $\neq 0$ & $\neq 0$ & $\neq 0$ \\
\hline
\end{tabular}
\end{table}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{nuclear_shapes.png}
\caption{A schematic show of some typical nuclear shapes. From left to right, the first row: (a) sphere, (b) prolate spheroid, (c) oblate spheroid, (d) hexadecapole shape; and the second row: (e) triaxial ellipsoid, (f) reflection a symmetric octupole shape, (g) tetrahedron, (h) reflection asymmetric octupole shape with very large quadrupole deformation and large hexadecapole deformation. Taken from [17].}
\end{figure}
\[ V = \alpha \rho + \delta_\lambda \Delta \rho \tau, \]

where \( \alpha, \rho, \delta_\lambda, \Delta, \rho, \tau \) are the expansion coefficients. In practical calculations, one should truncate the basis in a proper way [25, 26, 35].

The nucleus is assumed to be symmetric under the \( V_j \) group; that is, all the potentials and densities can be expanded as

\[ f_\rho (\varphi, z) = \sum f_\alpha (\varphi, z) \frac{1}{\sqrt{2\pi}} + \sum f_\alpha (\varphi, z) \frac{1}{\sqrt{2\pi}} \cos (2n\varphi), \]

where \( f_\rho (\varphi, z) = \sum f_\alpha (\varphi, z) \frac{1}{\sqrt{2\pi}} + \sum f_\alpha (\varphi, z) \frac{1}{\sqrt{2\pi}} \cos (2n\varphi), \]

3. Results and discussions

3.1. PES of actinides

In [25, 26], one- (1-d), two- (2-d), and three-dimensional (3-d) constrained calculations were performed for the actinide nucleus \( ^{240}\text{Pu} \). The MDC-RMF model with the parameter set PC-PK1 [38] was used. In figure 2 we show the 1-d potential energy curves from an oblate shape with \( V_j \) symmetry imposed: the red dashed curve is that with axial symmetry (AS) imposed, the green dotted curve that with reflection symmetry (RS) imposed, the violet dot-dashed line that with both symmetries (AS & RS) imposed. The empirical inner (outer) barrier height \( B_{\text{in}} \) (\( B_{\text{out}} \)) is denoted by the grey square (circle). The energy is normalized with respect to the binding energy of the ground state. The parameter set used is PC-PK1. Taken from [25].
shape. As $\beta_{20}$ further increases, the nucleus goes through a triaxial valley again, and then goes fission. The outer barrier is located at $\beta_{20} \approx 1.2120$, $\beta_{22} \approx 0.0222$, and $\beta_{30} \approx 0.3730$.

A systematic study of even−even actinide nuclei has been carried out and the results were presented in [26], where we have shown that the triaxial deformation lowers the outer barriers of these actinide nuclei by about $-0.51$ MeV (about $-10\%$ of the barrier height).

3.2. $Y_{32}$-correlations in $N = 150$ isotones

It has been anticipated that the tetrahedral shape ($\beta_{32} = 0$, if $\lambda \neq 3$ and $\mu \neq 2$) may appear in the ground states of some nuclei with special combinations of the neutron and proton numbers [9, 12, 16]. The tetrahedral symmetry-driven quantum effects may also lead to a large increase of binding energy in superheavy nuclei [39]. However, no solid experimental evidence has been found for nuclei with tetrahedral shapes. On the other hand, $\beta_{32}$ deformation may appear together with other shape degrees of freedom, say, $\beta_{20}$. For example, it has been proposed that the nonaxial octupole $Y_{32}$-correlation results in the experimentally observed low-energy $2^-$ bands in the $N = 150$ isotones [40] and the RASM calculations reproduce well the experimental observables of these $2^-$ bands [41].

In [42] the nonaxial reflection-asymmetric $\beta_{32}$ deformation in $N = 150$ isotones, namely $^{246}\text{Cm}$, $^{248}\text{Cf}$, $^{250}\text{Fm}$ and $^{252}\text{No}$, was investigated using the MDC-RMF model with the parameter set DD-PC1 [43]. It was found that due to the interaction between a pair of neutron orbitals, $\{734,9/2\}$ originating from $\nu j_{15/2}$ and $\{622,5/2\}$ originating from $\nu g_{9/2}$, and that of a pair of proton orbitals, $\{521,3/2\}$ originating from $\pi f_{7/2}$ and $\{633,7/2\}$ originating from $\pi i_{13/2}$, rather strong nonaxial octupole $Y_{32}$ effects appear in $^{248}\text{Cf}$ and $^{250}\text{Fm}$, which are both well deformed with large axial-quadrupole deformations, $\beta_{20} \approx 0.37$.

In figure 5, the potential energy curve, i.e. the total binding energy as a function of $\beta_{32}$, is shown for $^{248}\text{Cf}$. At each point of the potential energy curve, the energy is minimized automatically with respect to other shape degrees of freedom such as $\beta_{20}$, $\beta_{22}$, $\beta_{30}$ and $\beta_{40}$, and so forth. One finds in this curve a clear pocket with depth more than 0.3 MeV. As similar potential energy curve was also obtained for $^{250}\text{Fm}$. For $^{246}\text{Cm}$ and $^{252}\text{No}$, only a shallow minimum develops along the $\beta_{32}$ shape degree of freedom. It was also shown that the evolution of the nonaxial octupole $\beta_{32}$ effect along the $N = 150$ isotonic chain is not very sensitive to the form of the energy density functional and the parameter set we used [42].

Both the nonaxial octupole parameter $\beta_{32}$ and the energy gain due to the $\beta_{32}$-distortion reach maximal values at $^{248}\text{Cf}$ in the four nuclei along the $N = 150$ isotonic chain [42]. This is consistent with the analysis given in [41, 44] and the
experimental observation that in $^{248}$Cf, the $2^-$ state is the lowest among these nuclei [40]. These results indicate a strong $\gamma_3\gamma_5$-correlation in these nuclei.

4. Summary

In this paper we present the formalism and some applications of the multidimensionally constrained relativistic mean field (MDC-RMF) models in which all shape degrees of freedom $\beta_{\mu}$ with even $\mu$ are allowed. The potential energy surfaces (curves) of actinide nuclei and the effect of the triaxiality on the first and second fission barriers were investigated. It is found that besides the octupole deformation, the triaxiality also plays an important role for the second fission barriers. The nonaxial reflection-asymmetric $\beta_{32}$ shape in $N = 150$ isotones was studied, and rather strong nonaxial octupole $\gamma_{32}$ effects have been found in $^{248}$Cf and $^{280}$Fm, which are both well deformed with large axial-quadrupole deformations, $\beta_{20} \approx 0.3$.

Acknowledgments

This work has been supported by Major State Basic Research Development Program of China (Grant No. 2013CB834400), National Natural Science Foundation of China (Grant Nos. 11121403, 11175252, 11120101005, 1121120152 and 11275248), the Knowledge Innovation Project of Chinese Academy of Sciences (Grant No. KJCX2-EW-N01). The results described in this paper are obtained on the ScGrid of Supercomputing Center, Computer Network Information Center of Chinese Academy of Sciences.

References

[1] Bohr A and Mottelson B R 1998 Nuclear Structure vol 1
(Singapore: World Scientific)

[2] Ring P and Schuck P 1980 The Nuclear Many-Body Problem
(Berlin: Springer)

[3] Butler P A and Nazarewicz W 1996 Rev. Mod. Phys. 68
349–421

[4] Starosta K et al 2001 Phys. Rev. Lett. 86 971–4

[5] Odegard S W et al 2001 Phys. Rev. Lett. 86 5866–9

[6] Meng J and Zhang S Q 2010 J. Phys. G: Nucl. Phys. 37
064025

[7] Hamamoto I, Mottelson B, Xie H and Zhang X Z 1991
Z. Phys. D 21 163–75

[8] Skalski J 1991 Phys. Rev. C 43 140–5

[9] Li X and Dudek J 1994 Phys. Rev. C 49 1250–2

[10] Takami S, Yabana K and Matsuo M 1998 Phys. Lett. B 431
242–8

[11] Yamagami M, Matsuyanagi K and Matsuo M 2001 Nucl. Phys.
A 693 579–602

[12] Dudek J, Gozdz A, Schunck N and Miskiewicz M 2002 Phys.
Rev. Lett. 88 252502

[13] Dudek J, Curien D, Dubray N, Dobaczewski J, Pangon V,
Olbratowski P and Schunck N 2006 Phys. Rev. Lett. 97
072501

[14] Olbratowski P, Dobaczewski J, Powolowski P, Sadziak M and
Zberecki K 2006 Int. J. Mod. Phys. E 15 333–8

[15] Zberecki K, Magierski P, Heenen P H and Schunck N 2006
Phys. Rev. C 74 051302(R)

[16] Dudek J, Gozdz A, Mazurek K and Molique H 2010 J. Phys.
G: Nucl. Phys. 37 064032

[17] Lu B N 2012 Multi dimensional constrained relativistic mean
field theory and the potential energy surfaces and fission barriers of actinide nuclei PhD Thesis Institute of
Theoretical Physics, Chinese Academy of Sciences (in Chinese)

[18] Pashekevich V V 1969 Nucl. Phys. A 133 400–4

[19] Möller P and Nilsson S G 1970 Phys. Lett. B 31 283–6

[20] Girod M and Grammaticos B 1983 Phys. Rev. C 27 2317–39

[21] Rutz K, Maruhn J A, Reinhard P G and Greiner W 1995 Nucl.
Phys. A 590 680–702

[22] Abusara H, Afanasjev A V and Ring P 2010 Phys. Rev. C 82
044303

[23] Prassa V, Nikšić T, Lalazissis G A and Vretenar D 2012 Phys.
Rev. C 86 024317

[24] Prassa V, Nikšić T and Vretenar D 2013 Phys. Rev. C 88
044324

[25] Lu B N, Zhao E G and Zhou S G 2012 Phys. Rev. C 85
011301(R)

[26] Lu B N, Zhao J, Zhao E G and Zhou S G 2013 Phys. Rev. C 89
014302

[27] Serot B D and Walecka J D 1986 Adv. Nucl. Phys. 16 1–327

[28] Reinhard P G 1989 Rep. Prog. Phys. 52 439–514

[29] Ring P 1996 Prog. Part. Nucl. Phys. 37 193–263

[30] Vretenar D, Afanasjev A, Lalazissis G and Ring P 2005 Phys.
Rep. 409 101–259

[31] Meng J, Toki H, Zhou S G, Zhang S Q, Long W H and
Geng L S 2006 Prog. Part. Nucl. Phys. 57 470–563

[32] Nikšić T, Vretenar D and Ring P 2011 Prog. Part. Nucl. Phys.
66 519–48

[33] Lu B N, Zhao J, Zhao E G and Zhou S G 2012 EPJ Web Conf.
38 05003

[34] Lu B N, Zhao J, Zhao E G and Zhou S G 2014 J. Phys. Conf.
Ser. 492 012014

[35] Lu B N, Zhao E G and Zhou S G 2011 Phys. Rev. C 84 014328

[36] Gamblin Y K, Ring P and Thimet A 1990 Ann. Phys. 198
132–79

[37] Ring P, Gamblin Y K and Lalazissis G A 1997 Comput. Phys.
Commun. 105 77–97

[38] Zhao P W, Li Z P, Yao J M and Meng J 2010 Phys. Rev. C 82
054319

[39] Chen Y and Gao Z 2013 Nucl. Phys. Rev. 30 278–83

[40] Robinson A P et al 2008 Phys. Rev. C 78 034308

[41] Chen Y S, Sun Y and Gao Z C 2008 Phys. Rev. C 77
061305(R)

[42] Zhao J, Lu B N, Zhao E G and Zhou S G 2012 Phys. Rev. C 86
057304

[43] Nikšić T, Vretenar D and Ring P 2008 Phys. Rev. C 78 034318

[44] Jolos R V, Malov L A, Shirikova N Y and Sushkov A V 2011
J. Phys. G: Nucl. Part. Phys. 38 115103