RPE | Radiation Physics & Engineering
An International Peer-Reviewed Journal
Published by K.N. Toosi University of Technology
http://rpe.kntu.ac.ir
Research Article

Radiation Physics and Engineering 2021; 2(2):1–6
https://doi.org/10.22034/rpe.2021.257743.1027

Nuclear deformation parameters of Sn isotopes

Mahdieh Ghafouri*, Hossein Sadeghi
Department of Physics, Faculty of Science, University of Arak, Arak 8349-8-38156, Iran

HIGHLIGHTS

- TDHF method as a function of time for a set of Sn isotopes has been studied
- We study skyrm forces with quadrupole spectra along the Sn isotope chains.
- We applied the Sky3D to solve static (dynamic) equations.
- The effective interaction plays an important role in the details of carries information about the heavy-ion reactions.

ABSTRACT

The mean-field model based on Skyrm Forces (SF) or associated density function has a wide application to describe nuclear states, collective vibrational excitation, and heavy-ion collisions. The Sky3D solves static or dynamic equations on a Cartesian 3-D mesh with isolated or periodic boundary conditions without further assumptions on the symmetry which shows more characteristics of the structure of nuclei. In the present work, time-dependent Hartree-Fock Skyrm (TDHF) calculations were completed on a set of Sn isotopes to obtain and compare the nuclear deformation parameters in static and dynamic states. It was found that in deficient neutron nuclei, even the most modern particle calculations unable to describe the improved collectivity below the mean shell in Sn approaching $N = Z = 50$. It was shown that the effective interaction plays an important role in the details of the reaction, and carries information about the heavy-ion reactions to the details of the effective interaction.

KEYWORDS

Hartree-Fock Skyrm Method
Density Function Theory
Skyrm Forces
Heavy-Ion
Deformation Parameters

HISTORY

Received: 18 November 2020
Revised: 13 June 2021
Accepted: 17 June 2021
Published: Spring 2021

1 Introduction

Self-Consistent Mean Field (SCMF) models express the desired single-body potential by Single-Particle (SP) wave functions. SCMF is specifically the Hartree-Fock (HF) theory in which the functions of SP waves are determined differently by a dipole interaction (Fetter and Walecka, 2012; Maruhn et al., 2010). Studying and describing dynamic processes is more important than modeling or structural design. Among these models, SCMF is the first model of choice in this field. The developed HF model is the Time-Dependant HF (TDHF), introduced at the beginning of the 1930s (Dirac, 1930). Among the theoretical methods used to study heavy-ion reactions, TDHF models have recently obtained sufficient full implementation status of limited approximations and acted at an appropriate speed in a way that systematically changing effective interactions in calculations is possible. Moreover, by increasing the computer capacities, large-scale TDHF calculations have been possible in recent decades.

Nuclear TDHF began about forty years ago and was developed as a powerful and immersive tool to simulate a wide range of dynamic processes (Bonche et al., 1976). The dynamics of heavy-ion collisions within the TDHF developed by Simenel and Umar (Simenel and Umar, 2018). This work presents studies on low-energy heavy-ion reactions and examines the significant effects on observations of the shape of spin-orbit interaction, the tensor force, and the time-dependent density functions (Stevenson and Barton, 2019). The effective interaction in the dynamics of heavy-ion reactions plays an important role in the understanding of the reaction details. In the case of the Tensor-Skyrm interaction, the structures of individual nuclei and their dynamics in collisions may be affected.

For TDHF calculations, a code based on the Skyrm energy function is used. This code, named Sky3D, solves static or dynamic equations on a three-dimensional Cartesian space with isolated (periodic) or periodic boundary conditions and without hypotheses with additional symmetry (Maruhn et al., 2014; Hashimoto and Nodeki, 2007). This code implements equations based on the Skyrm energy function and determines the base state structure of

*Corresponding author: Mahdieh.ghafouri@yahoo.com

nuclei by the static version of the equations. Using models that show more features of the structure of nuclei, a better understanding of the structure of nuclei can be achieved. The pairing can be included in the BCS approximation in the static case. The boundary conditions for wave functions are always periodic, while the potential can also be calculated for an isolated charge distribution.

In the present work, we study Skyrm forces with quadrupole spectra along the Sn isotope chains. This article is part of the Functional Universal Nuclear Energy Density Project (UNEDF), which complements the calculation of heavy-nuclear calculations. This code includes both dynamic and static calculations. The spatial distribution of nuclear material in atomic nuclei has become a fundamental characteristic of the study of nuclear physics. The number of experiments that permit the study of atomic nucleus forms is constantly increasing. In this work, a very significant case of nuclear quadrupole deformation is discussed and are compared with those of the theatrical results.

The article is organized as follows: In section 2, we briefly present the basic ideas and the theoretical framework, and we describe how we obtain the various observable presented in the work. In section 3, we report our results which obtained for a set of Sn isotopes and compare nuclear deformation parameters in static and dynamic states. In section 4, we summarize our results and present the conclusions.

2 Brief review of purpose and structure

2.1 The time-dependent Hartree-Fock

The stationary equations are obtained by considering the single-particle wave functions ψ_α mean-field equations as

$$\widehat{H}\psi_\alpha = \varepsilon_\alpha \psi_\alpha \tag{1}$$

where $\widehat{H}$ is the mean-field Hamiltonian, and ε_α is the single-particle energy.

In the static calculations, there are limitations that the most application are used in a quadrupole restricted by expectation value $\langle\psi_\alpha|H-\lambda Q_{20}|\psi_\alpha\rangle$. By adding a constraint that includes a potential sentence in single-particle Hamiltonian, for example, in the case of quadrupole, we obtain:

$$\widehat{H} \;\rightarrow\; \widehat{H} - \lambda(2z^2 - x^2 - y^2) \tag{2}$$

As it is known, the applied numerical method does not limit the deformation. Therefore, one should be careful of unstable constraints such as quadrupole which can reach large values at the edges of the computing box and may pull the wave function there (Rutz et al., 1995).

In the time-dependent Schrodinger equation (Koonin, 1975; Rowe et al., 2020), we see

$$i\hbar\frac{\partial}{\partial t}|\psi_\alpha\rangle = \widehat{H}|\psi_\alpha\rangle \tag{3}$$

Also, we can define the Hamiltonian of the interaction as follows

$$\widehat{H} = \widehat{T} + \widehat{V} = \sum_{\alpha\beta} t_{\alpha\beta} a^\dagger_\alpha a_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \tag{4}$$

where $t_{\alpha\beta}$ is the kinetic energy and $V_{\alpha\beta\gamma\delta}$ is the two-body interaction matrix elements. Moreover, $a^\dagger_i$ and a_i create and annihilate a particle in the state i, respectively.

The TDHF equation is

$$S = \int \mathrm{d}t\Big[E[\{\psi_\alpha\}] - \sum_\alpha \langle\psi_\alpha|i\partial_t|\psi_\alpha\rangle\Big] \tag{5}$$

The mean-field equations used in the code are based on the widely Skyrme energy functional. For recent reviews, see (Erler et al., 2011; Bender et al., 2003). Threfore,

$$\begin{aligned} E_{tot} =& T + (E_0 + E_1 + E_3 + E_{ls}) \\ &+ E_{Coulomb} + E_{pair} + E_{corr} \end{aligned} \tag{6}$$

In this equation, there is a set of sentences derived from the Skyrme force. For more details, see (Maruhn et al., 2014). TDHF can be solved as

$$\begin{aligned} |\psi_\alpha(t+\Delta t)\rangle &= U(t, t+\Delta t)\,|\psi_\alpha(t)\rangle \\ U(t, t+\Delta t) &= \widehat{T}\exp\Big[-\frac{i}{\hbar}\int_t^{t+\Delta t}\widehat{H}(t')\mathrm{d}t'\Big] \end{aligned} \tag{7}$$

where $\widehat{U}$ and $\widehat{T}$ are the time-evolution and the time-ordering operations, respectively.

Also, the extension of the Skyrme energy is displayed as

$$\begin{aligned} E_{tot,HF} &= \frac{1}{2}\sum_\alpha (t_\alpha + E_\alpha) + E_{3,corr} + E_{C,corr} \\ E_{3,corr} &= \int \mathrm{d}^3r\,\frac{\alpha}{6}\rho^\alpha\Big[b_3\rho^2 - b_3'(\rho_P^2 + \rho_n^2)\Big] \\ E_{C,corr} &= \frac{1}{4}(\frac{3}{\pi})^{1/3}\int \mathrm{d}^3r\,\rho_{pr}^{4/3} \end{aligned} \tag{8}$$

where ρ is the local density:

$$\rho_q(r) = \sum_{\alpha\in q}\sum_s \nu_\alpha^2 |\psi_\alpha(r,s)|^2 \tag{9}$$

where for protons, $q = p$, and for neutrons, $q = n$. $\rho = \rho_p + \rho_n$ is the total density. b_3 is defined according to the t and x coefficients that is in definition Skyrme-force. For more details, see (Maruhn et al., 2014). In this code, the total energy is computed through Eqs. (6) and Eq. (8). In calculating the total energy, we use a three-dimensional solver (Skyrme-TDHF) which solves the self-consistent HF equation and the TDHF equation.

2.2 Quadrupole resonance in Sn

To investigate the vibrational dynamics of a nucleus, we first observe quadrupole oscillations in Sn. Afterwards, the quadrupole resonance spectra are obtained. In a large pulse, some energies can be excited, while in an extremely short pulse, an immediate increase is observed. It is an appropriate system to analyze excited spectra. It allows complete spectral analysis. Though the excited spectrum is one of the most elementary features of the system, there are also many interesting dynamic features. The quadrupole spectra of the present Sn isotopes are well represented in the resonance region. In heavy cores, there are peaks which their intensity are lower than a few MeV. These low intensity parts of the spectrum should be considered for non-magical cores.

2.3 Multipole moment

In this TDHF calculation, we use the Skyrm SLy6 interaction for nucleons in the mean field Hamiltonian. Numerical calculations are performed on a Cartesian three-dimensional grid. The study of the low-energy properties of even-even isotopes of existing nuclei, including Sn, is the subject of many experimental studies. A significant number of the density distribution properties are characterized by multipole moments. The most important one is the center of mass (c.m.). For the quadrupole state, spherical moments are defined as follows:

$$Q_{2m}^{type} = \int \mathrm{d}^3 r \; r^2 Y_{2m} \rho^{(type)}(\vec{r} - \vec{R}) \tag{10}$$

In this code, the Cartesian quadrupole reads

$$Q = 2\sin(\frac{\pi z}{z_{box}})^2 - \sin(\frac{\pi y}{y_{box}})^2 - \sin(\frac{\pi x}{x_{box}})^2 \tag{11}$$

There are two shape parameters a_0 and a_2, called as deformation β and triaxiality γ. These are known as Bohr-Mottelson parameters:

$$\begin{aligned} \beta &= \sqrt{a_0 + 2a_2^2} \\ \gamma &= a\tan\Big(\frac{\sqrt{2}a_2}{a_0}\Big) \end{aligned} \tag{12}$$

More detailed energy observations are provided by single particle energies. Also, the deformation parameter is calculated in terms of transition probability as follows (Raman et al., 2001):

$$\beta = [B(E2)\uparrow]^{1/2}[3ZeR_0^2/4\pi]^{-1} \tag{13}$$

In this equation, Z stands for the atomic number, and R_0 is the average radius of the nucleus.

3 Results and discussion

In the present work, we examine the properties of giant quadrupole resonance in tin isotopes. We also use the Skyrm SLy6 force to describe the isotopic properties of the kernel corresponding to the stability line β for the drip lines. A long sampling time of 5000 fm.c^{-1} suffices to display giant resonance. The resonance intensity is well concentrated within an area, but it is divided into several sub-peaks. The general location of the resonance area is very important. However, it is worthy to mention that details should also be taken into account.

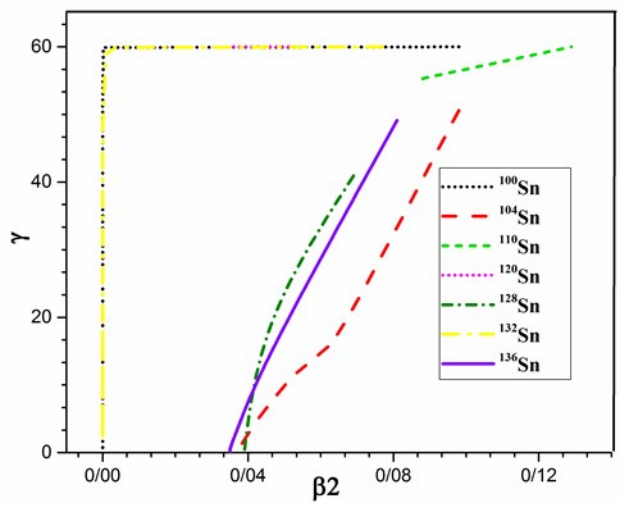

Figure 1: Scattering of gamma versus beta for tin isotopes.

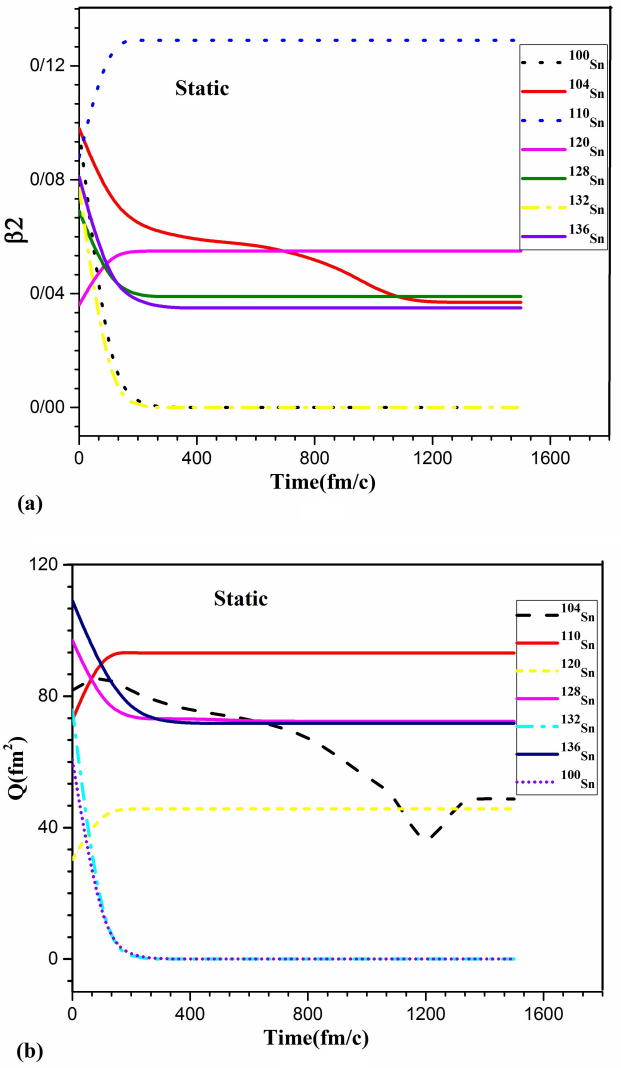

Figure 2: Time evolution of the quadrupole moments and beta variations for tin isotopes for static state.

As Fig. 1 shows, the beta (β) and gamma (γ) distortion parameters decrease during the time. By increasing the scattering angle, the greatest deformation occurs. As

Table 1: Comparison between the theoretical results and the present work.

Isotope	$B(E2)e^2b^2$				b (our work)
Sn-104	(Doornenbal et al., 2014) 0.163(26)	(Guastalla et al., 2013) 0.10(4)	(Bader et al., 2013) 0.180(37)	Our work 0.0197	0.037

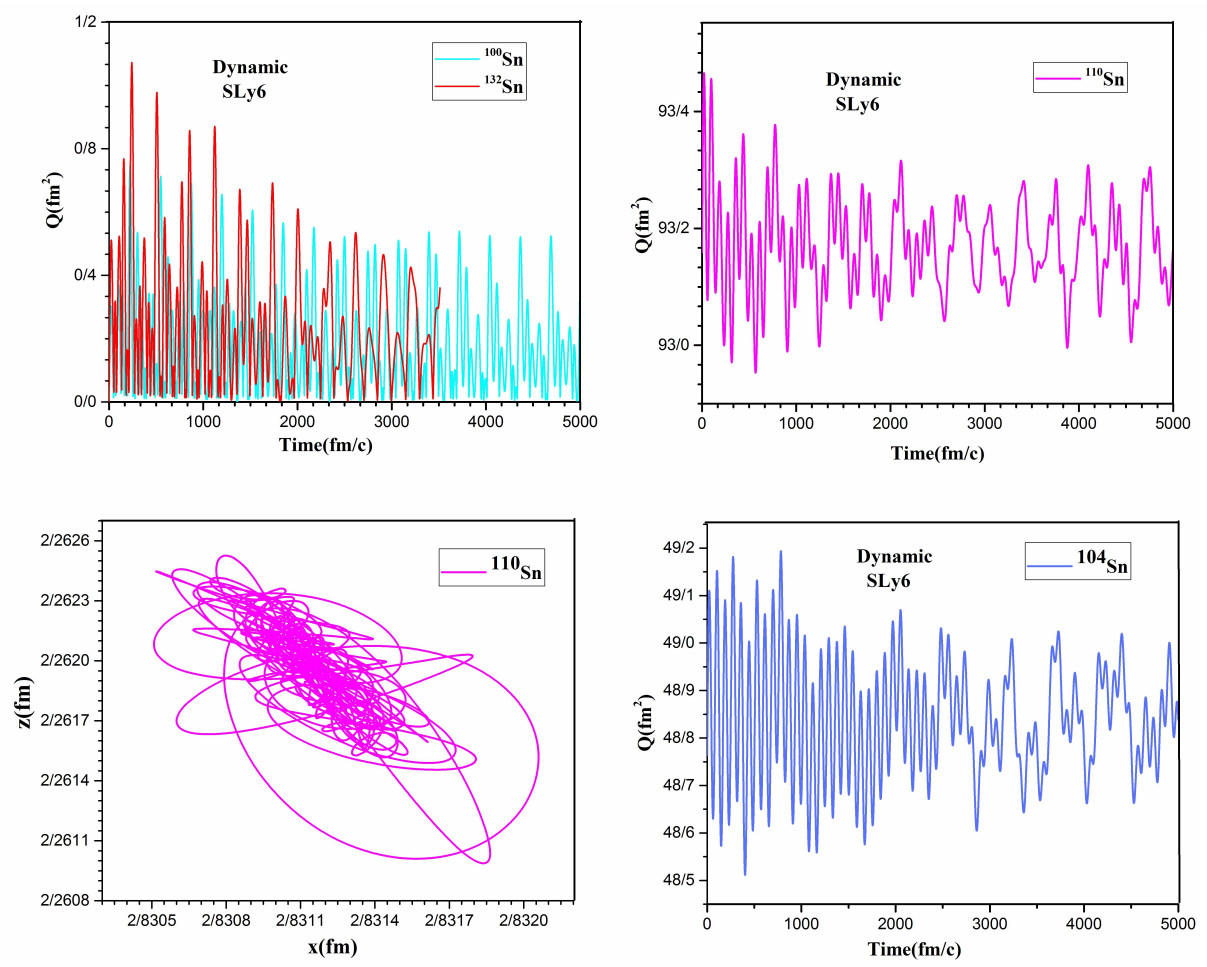

Figure 3: Time evolution of the quadrupole momentum from TDHF calculations in dynamic mode for tin isotopes and time changes in the $x-z$ plane for Sn-110.

mentioned before, Beta and gamma are the deformation parameters of Bohr-Mottelson. These values are calculated only for the total weight distribution. Beta is dimensionless and gamma is presented in degrees. The scatter of gamma versus beta is shown in this figure. In the magical elements of Sn-100 and Sn-132, the scattering changes are very small. However, by moving away from the magic numbers with the shell closed and being in different spin and orbital states, these changes are obvious, especially for Sn-110. In the rest of the sample, gamma dispersion is near zero with a decrease in beta.

In Fig. 2, quadrupole moments and beta changes for a range of tin isotopes for the static state are compared. As this figure shows, for the elements with closed and magical shells, the quadrupole moments are zero and most of them belong to Sn-110. For Sn isotopes that are neutron deficient (for example, Sn-104), the results show that the departure from large-scale shell-model calculations that is to originate for the interplay of proton particle-hole configurations persists. It affects the quadrupole collectivity in isotopes that are in proton-magic isotope chains. There is no specific fluctuation here. Also, it is worth noting that proton states are driven to slightly higher energies by the Coulomb force. Static calculus takes a few minutes using a modern computer. The output of the state properties of only one particle should be noted (see Appendix 1).

In Table 1, the quadripolar deformation parameter of the theoretical results and the present work for Sn-104 according to $B(E2)$, defined in Eq (13), are compared.

In these diagrams, in Fig. 3, quadrupole moments are plotted dynamically. And many resonances are visible even in Sn-100 and Sn-132 elements. The highest moments of the dynamic state are Sn-110 and the weakest at Sn-100 and Sn-132.

Figure 4 shows the variations of the quadrupole impulse with respect to energy in dynamic mode. In giant resonance (GR), the excited states of the nucleus have been widely studied (Goeke and Speth, 1982). Skyrme

forces, if selected properly, can provide a good explanation for them (Bender et al., 2003; Klüpfel et al., 2009). Given that RG is associated with nuclear dynamics, TDHF is a good starting point for describing them.

It should be noted that the analysis of two bodies is valid only if the reaction plane is $x - z$, and the printed results may not be useful if the physical situation is not of a two-body nature.

Sample data on tin isotopes are Sn-104 and Sn-110. It can be clearly seen that the static deformation of these isotopes is very different from that of isotopes close to magic numbers, and their dynamic deformation, defined by the probability of $E2$ transfer, is very high. Taking into account the hypotheses of this work, this fact shows that the deformation of this core sample is very vibratory. In recent years, sum rules are more interested in the possibility of obtaining simple expressions for some of the intermediate properties of the collective excitation spectrum which analytically allow a very clear study; Though it is sometimes independent of the model and the systematic properties such as the dependence of excitation energies and so on. Moreover, other collective theories such as macroscopic models and generator coordinate methods, can be systematically linked to tRPA by summation rules.

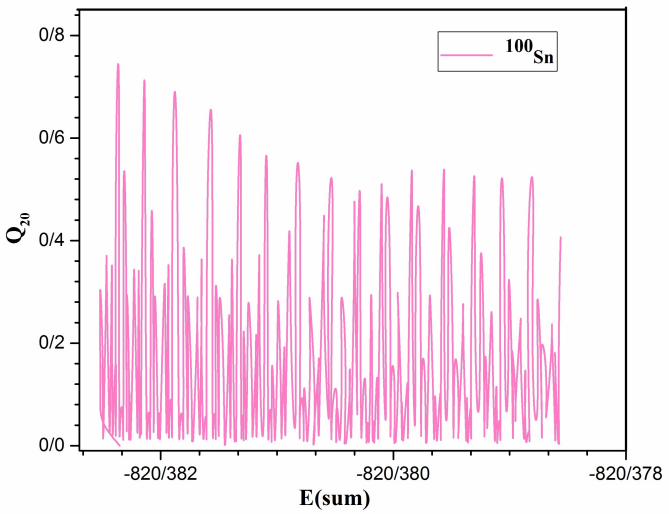

Figure 4: Variations in quadrupole momentum relative to energy for the present test case of Sn-100 and Sn-110 computed with the forces SLy6.

4 Summary and Conclusion

The Sk3D code is used here (Maruhn et al., 2014). In this work, it is shown that the nucleons which quadrupole deformation parameters are inferred from the data related to quadrupole momentum (Q) and the probability of quadrupole electric transfer are divided into several groups. The data take into account both static deformation and dynamic deformation due to vibration of the nuclear surface in the ground state. The comparison of static and general deformations makes it possible to obtain data on nuclear properties. We have tried to choose isotope samples that are both loose and rigid. Experimental work has been conducted on a small number of isotopes to date, which is fortunately increasing. Because of the new composition of the isotopes, this set was used to produce a variety of nuclear forms.

In this work, the calculations of the TDHF method as a function of time for a set of Sn isotopes have been obtained. Moreover, the parameters of nuclear deformation in static and dynamic states of Sn-104 have been compared. It was found that in defective neutron nuclei, even the most modern particle calculations are not able to describe the improved community under the central shell in Sn approaching $N = Z = 50$. The authors are developing this work.

Appendix 1. Module Parameters

This module contains general parameters essential for checking the code, as well as the mathematical and physical constants that generally are used.

nx, ny, nz, dx, dy, dz: define the box for the nucleus.

nprot, nneut: number of protons and neutrons (Z and N).

npsi(1) for neutrons, **npsi(2)** for protons: to add some unoccupied wave functions.

nt: the number of time steps, and **psi** the number of wave functions.

radin[x,y,z]: radii for the oscillator initialization.

mprint: control for printer output. If mprint is greater than zero, more detailed output is produced every mprint iterations or time steps on standard output.

mplot: if mplot is greater than zero, a printer plot is produced and the densities are dumped onto *.tdd files every mplot time steps or iterations.

mrest: if greater than zero.

wffile: is produced every mrest iterations or time steps .

out.txt: contains the full print output.

sky3d.seq > out.txt: produces the output in "out.txt".

References

Bader, V., Gade, A., Weisshaar, D., et al. (2013). Quadrupole collectivity in neutron-deficient Sn nuclei: Sn-104 and the role of proton excitations. *Physical Review C*, 88(5):051301.

Bender, M., Heenen, P.-H., and Reinhard, P.-G. (2003). Self-consistent mean-field models for nuclear structure. *Reviews of Modern Physics*, 75(1):121.

Bonche, P., Koonin, S., and Negele, J. (1976). One-dimensional nuclear dynamics in the time-dependent hartree-fock approximation. *Physical Review C*, 13(3):1226.

Dirac, P. A. (1930). Note on exchange phenomena in the Thomas atom. In *Mathematical Proceedings of the Cambridge Philosophical Society*, volume 26, pages 376–385. Cambridge University Press.

Doornenbal, P., Takeuchi, S., Aoi, N., et al. (2014). Intermediate-energy Coulomb excitation of Sn-104: Moderate E2 strength decrease approaching Sn-100. *Physical Review C*, 90(6):061302.

Erler, J., Klüpfel, P., and Reinhard, P. (2011). Self-consistent nuclear mean-field models: example Skyrme–Hartree–Fock. *Journal of Physics G: Nuclear and Particle Physics*, 38(3):033101.

Fetter, A. L. and Walecka, J. D. (2012). *Quantum theory of many-particle systems*. Courier Corporation.

Goeke, K. and Speth, J. (1982). Theory of giant resonances. *Annual Review of Nuclear and Particle Science*, 32(1):65–115.

Guastalla, G., DiJulio, D., Górska, M., et al. (2013). Coulomb excitation of Sn-104 and the strength of the Sn-100 shell closure. *Physical Review Letters*, 110(17):172501.

Hashimoto, Y. and Nodeki, K. (2007). A numerical method of solving time-dependent Hartree-Fock-Bogoliubov equation with Gogny interaction. *arXiv preprint arXiv:0707.3083*.

Klüpfel, P., Reinhard, P.-G., Bürvenich, T., and thers (2009). Variations on a theme by Skyrme: A systematic study of adjustments of model parameters. *Physical Review C*, 79(3):034310.

Koonin, S. E. (1975). *Hydrodynamic approximations to time-dependent Hartree-Fock*. PhD thesis, Massachusetts Institute of Technology.

Maruhn, J. A., Reinhard, P.-G., Stevenson, P., et al. (2014). The tdhf code sky3d. *Computer Physics Communications*, 185(7):2195–2216.

Maruhn, J. A., Reinhard, P.-G., and Suraud, E. (2010). *Simple models of many-fermion systems*. Springer Science & Business Media.

Raman, S., Nestor Jr, C., and Tikkanen, P. (2001). Transition probability from the ground to the first-excited 2+ state of even–even nuclides. *Atomic Data and Nuclear Data Tables*, 78(1):1–128.

Rowe, D. J., Trainor, L. E., and Wong, S. S. (2020). *Dynamic structure of nuclear states*. University of Toronto Press.

Rutz, K., Maruhn, J., Reinhard, P.-G., et al. (1995). Fission barriers and asymmetric ground states in the relativistic mean-field theory. *Nuclear Physics A*, 590(3-4):680–702.

Simenel, C. and Umar, A. (2018). Heavy-ion collisions and fission dynamics with the time-dependent Hartree–Fock theory and its extensions. *Progress in Particle and Nuclear Physics*, 103:19–66.

Stevenson, P. and Barton, M. (2019). Low-energy heavy-ion reactions and the Skyrme effective interaction. *Progress in Particle and Nuclear Physics*, 104:142–164.