CALCULATION OF POTENTIAL ENERGY SURFACES FOR LIGHT NUCLEI IN β-γ PLANE

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Abstract

The nuclei having asymmetric shapes in their ground state have now become an interesting topic in both theoretical and experimental nuclear structure physics. In my present work, the deformations in neutron-rich light-mass nuclei are investigated by using self-consistent mean field approach. Using the constrained Skyrme Hartree-Fock+BCS method on the three-dimensional Cartesian mesh, we calculated the potential energy surfaces (PES) for some selected light nuclei (^{16}O, ^{22}Ne and ^{28}Si) in $\beta-\gamma$ plane where β represents ellipsoidal quadrupole deformation and γ, the degree of axial asymmetry.

Keywords: light nuclei, Hartree-Fock + BCS method

Introduction

One of the major challenges in nuclear physics is the study of the nuclear structures of nuclei which can provide the precious information in nuclear theory. In the past decades, the relativistic and non-relativistic self-consistent mean-field approaches have been popular to study the structure of nuclei. In this report, we choose the non-relativistic mean field theory and calculate their potential energy surfaces to verify the shapes of ^{16}O, ^{22}Ne and ^{28}Si nuclei.

The shape of a deformed nucleus can be parameterized by representing the nuclear surface via expansion of the spherical harmonics, $Y(\theta,\phi)$, as follow:

$$R(\theta,\phi)=R_0\left(1+\sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{\lambda}\alpha_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi)\right) \tag{1}$$

where $R(\theta,\phi)$ denotes the nuclear radius in the direction (θ,ϕ), λ indicates the order of the expansion, R_0 is the radius of a sphere containing the same

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total volume and $\alpha_{\lambda\mu}$ the expansion coefficients describe the variations of the nuclear shape with different multipolarity around the ground state.

In my calculation, the quadrupole deformation (λ=2) which is the most important deviation from spherical shape is taken into account. For the case of pure quadrupole deformation, the Eq. 1 is given by

$$R(\theta,\phi)=R_0\left(1+\sum_{\mu=-2}^{2}\alpha_{2\mu}Y_{2\mu}(\theta,\phi)\right) \tag{2}$$

Such quadrupole shapes can either have axial symmetry, in which case one distinguishes elongated (prolate) and flattened (oblate) shapes, or the deformation can be without axial symmetry resulting in different elongations along the three axes of the system, referred to as triaxial shape.

There is a set of parameters introduced by Bohr [1] which corresponds to something like polar coordinates in space of $(\alpha_{20},\alpha_{22})$ and is defined by

$$\alpha_{20}=\beta_2\cos\gamma, \tag{3}$$

$$\alpha_{22}=\frac{1}{\sqrt{2}}\beta_2\sin\gamma, \tag{4}$$

where the parameters β_2 and γ represent the deformation and non-axiality of the nuclear shapes, respectively.

The aim of this present work is to study the shapes of light nuclei (^{16}O, ^{22}Ne, ^{28}Si) using self-consistent mean field approach. The structures of these nuclei will be investigated by calculating the potential energy surfaces in beta-gamma ($\beta-\gamma$) plane which can clearly show the structure of nuclei. Then Ev8 program which solves the Skyrme-Hartree-Fock+BCS problem using a 3-dimensional Cartesian mesh will be employed in this calculation [2].

Formalism

I. Hartree-Fock Equations with Skyrme Interaction

The aim of the Hartree-Fock method is to approximate the two-body Hamiltonian operator as an effective single-particle potential. The full many-

body Hamiltonian can be written in terms of a one-body kinetic energy term and a two-body force as follows

$$H = \sum_{i=1}^{N} \hat{t}_i + \frac{1}{2} \sum_{i \neq j}^{N} \hat{V}\left(r_i, r_j\right) \tag{5}$$

where the first term is the usual kinetic energy operator, and the second is the two-body force including the Coulomb interaction. The simplified expression for the Hatree-Fock equations is obtained

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + \int d\mathbf{r}' \, \rho(\mathbf{r}') \, V(\mathbf{r}, \mathbf{r}') \right) \varphi_i(\mathbf{r}) - \int d\mathbf{r}' \, \rho(\mathbf{r}, \mathbf{r}') \, V(\mathbf{r}, \mathbf{r}') \, \varphi_i(\mathbf{r}') = \varepsilon_i \, \varphi_i(\mathbf{r}). \tag{6}$$

This equation is known as the Hartree-Fock equation. The Hartree-Fock method is useful one because it gives an introduction to the solution of many-particle system and to the concepts of self-consistent field. In the following, the Skyrme approximation which can greatly reduce the number of integrations over single particle states will be discussed.

In non-relativistic approach, the most famous effective nucleon-nucleon interaction is the Skyrme type which was performed by Vautherin and Brink [3] has been used for this work. In the Skyrme-Hartree-Fock approach, the total binding energy of the system is given by the sum of the kinetic and Coulomb energies as well as the Skyrme energy functional that models the effective interaction between nucleons [4].

The full Skyrme interaction can be shown in the form of the following equation,

$$E = E_{Coulomb} + E_{kin} + E_{Sk} \, . \tag{7}$$

A Skyrme force that consists of central, spin-orbit and tensor interactions is given by

$$\hat{V}_{sk}(\mathbf{r}, \mathbf{r}') = \hat{V}^{central}(\mathbf{r}, \mathbf{r}') + \hat{V}^{LS}(\mathbf{r}, \mathbf{r}') + \hat{V}^{tensor}(\mathbf{r}, \mathbf{r}') \tag{8}$$

The Skyrme energy (E_{Sk}), is derived by evaluating,

$$E_{Sk} = \frac{1}{2} \sum_{i,j}^{A} \int \phi_i^*(\mathbf{r}') \phi_j^*(\mathbf{r}') \, \hat{V}_{sk}(\mathbf{r}, \mathbf{r}') \left(1 - \hat{P}_M \hat{P}_\sigma \hat{P}_q\right) \phi_i(\mathbf{r}) \, \phi_j(\mathbf{r}) \, d\mathbf{r} \, d\mathbf{r}' \big|_{\mathbf{r}=\mathbf{r}'} \tag{9}$$

where $\hat{P}_M$ is position exchange operator and $\hat{P}_q$ is isospin exchange operator. Finally, the result of the Skyrme interaction is given by

$$E_{Sk} = B_1\rho^2(\mathbf{r}) + B_2\sum_q \rho_q^2(\mathbf{r}) + B_3\left\{\rho(\mathbf{r})\tau(r) - j^2(\mathbf{r})\right\} + B_4\sum_q\left\{\rho_q(\mathbf{r})\tau_q(\mathbf{r}) - j_q^2(\mathbf{r})\right\}$$

$$+ B_5\rho(\mathbf{r})\nabla^2\rho(\mathbf{r}) + B_6\sum_q \rho_q(\mathbf{r})\nabla^2\rho_q(\mathbf{r}) + B_7\rho^\alpha(\mathbf{r})\rho^2(\mathbf{r}) + B_8\rho^\alpha(\mathbf{r})\sum_q \rho_q^2(\mathbf{r})$$

$$+ B_9\left[\rho(\mathbf{r})\nabla.J(\mathbf{r}) + S(\mathbf{r}).(\nabla\times j(\mathbf{r})) + \sum_q\left\{\rho_q(\mathbf{r})\nabla.J_q(\mathbf{r}) + S_q(\mathbf{r}).(\nabla\times j_q(\mathbf{r}))\right\}\right]$$

$$+ B_{10}S^2(\mathbf{r}) + B_{11}\sum_q S_q^2(\mathbf{r}) + B_{12}S^2(\mathbf{r})\rho^\alpha(\mathbf{r}) + B_{13}\rho^\alpha(\mathbf{r})\sum_q S_q^2(\mathbf{r})\rho_q^\alpha(\mathbf{r})$$

$$+ B_{14}\left(S(\mathbf{r}).T(\mathbf{r}) - J^2(\mathbf{r})\right) + B_{15}\left(S(\mathbf{r})\nabla^2 S(\mathbf{r})\right)$$

$$+ B_{16}\sum_q\left(S_q(\mathbf{r}).T_q(\mathbf{r}) - J_q^2(\mathbf{r})\right) + B_{17}\sum_q S_q(\mathbf{r})\nabla^2 S_q(\mathbf{r}) \qquad (10)$$

The Skyrme interaction enormously simplifies the calculations with its zero-range form and has been very successfully used to describe the masses, charge radii and excited states of finite nuclei.

II. Constrained Hartree-Fock Method

The map of the energy surface as function of quadrupole deformation can be obtained by imposing constraints on the axial and triaxial mass quadrupole moments in the Hamiltonian. There can be many cases where it may be desirable to calculate other points on the energy surface. In this work, constrained Hartree-Fock (CHF) method is used to calculate the energy surface as a function of collective parameters of "q" such as quadrupole deformation. In this method, a wave function such as $|\Phi(q)\rangle$ is used to minimize the total energy under the constraint that a certain single particle operator $\langle\hat{Q}\rangle$ which has a fixed expectation value

$$\langle H'\rangle = \langle H\rangle - \lambda\langle\hat{Q}\rangle, \text{ where } q = \langle\Phi|\hat{Q}|\Phi\rangle. \qquad (11)$$

Results and Discussion

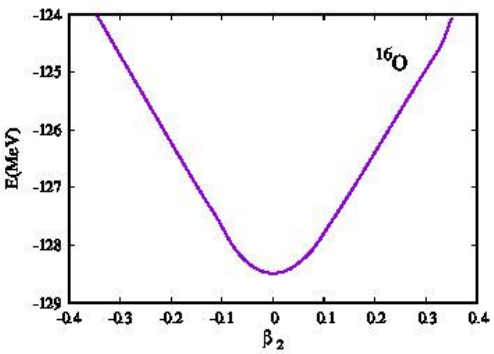
In this calculation, constrained quadrupole moment is added to the Hamiltonian to generate energy surfaces. The *Sly 4* parameter set is chosen for this calculation. Moreover, Ev8 code is used to solve the mean-field equations for the Skyrme energy density functional. In this code, the single particle wave functions are discretized on a 3-dimensional (3D) mesh to solve the mean-field equations.

A representation in terms of the deformation parameter (q) and the triaxiality angle (γ) is used to describe the shapes of nuclei. Their relationship can be represented by the following equations

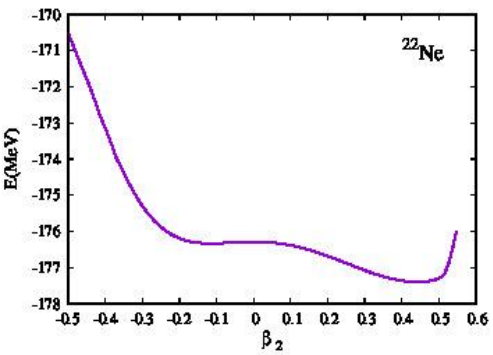
$$q_1 = q\cos(\gamma) - \frac{1}{\sqrt{3}} q\sin(\gamma) \tag{12}$$

$$q_2 = \frac{2}{\sqrt{3}} q\sin(\gamma). \tag{13}$$

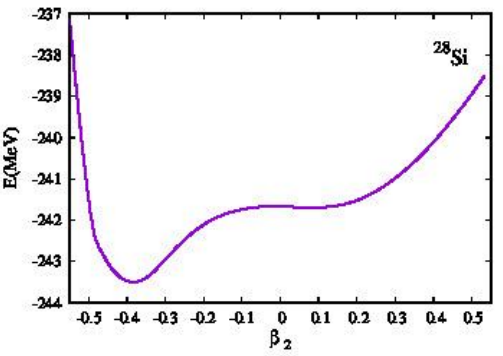
We select three light nuclei (^{16}O, ^{22}Ne and ^{28}Si) and calculate their potential energy surfaces. In order to know the shapes of these nuclei, the calculated potential energy surfaces as the function of deformation parameters are depicted in the following figures.



(a)



(b)



(c)

Figure 1: The potential energy surfaces as the function of deformation parameter (β) for (a) ^{16}O (b) ^{22}Ne and (c) ^{28}Si obtained with the *Sly4* parameter set.

For these calculations, we use the same symmetry axis for prolate and oblate configurations. The minimum energy located at the positive deformation parameter describes the prolate shape while the minimum energy with negative deformation parameter stands for the oblate shape. Fig. 1 (a) is the potential energy surface of ^{16}O nucleus which shows the well deep spherical configuration of the magic number. Its ground state energy is predicted to have -128.29 MeV at the origin. As can be seen in Fig. 1(b), there is the deep energy minimum of prolate configuration for ^{22}Ne which has the ground state energy of -177.17 MeV at $\beta = 4.7$. In Fig. 1(c), the PES of ^{28}Si nucleus shows the oblate configuration with ground state energy (-243.29 MeV) and its quadrupole deformation is -0.38.

In order to investigate whether there is deviation from axial symmetry in these nuclei, it is necessary to calculate their potential energy surfaces in $\beta - \gamma$ plane.

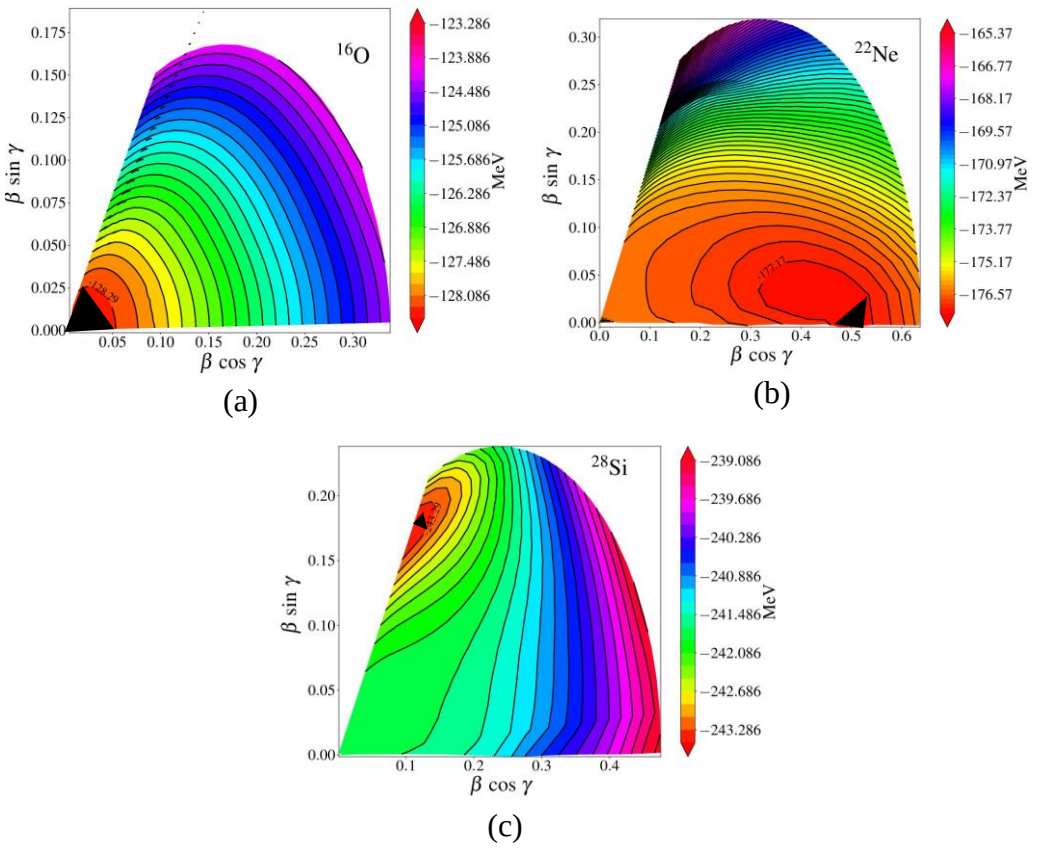


Figure 2: The potential energy surfaces of (a) ^{16}O (b) ^{22}Ne and (c) ^{28}Si in the $\beta-\gamma$ plane obtained with the *Sly4* parameter set.

To this end, we plotted the potential energy surfaces of three even-even nuclei, ^{16}O, ^{22}Ne and ^{28}Si in $\beta-\gamma$ plane as shown in Fig. 2. These contours are iso-energy lines, at every 0.2 MeV related to the ground state. In these figures, β represents the magnitude of deformation. The triaxiality angle $\gamma=0^{\circ}$ corresponds to prolate shapes, whereas $\gamma=60^{\circ}$ to oblate shape and triaxial for $0^{\circ}<\gamma<60^{\circ}$. The potential energy surface (PES) for the ^{16}O nucleus in the (β,γ) plane is plotted in Fig. 2(a). It has the minimum energy at the origin showing that it has the nature of spherically symmetric. Fig. 2(b) indicates ^{22}Ne nucleus is prolately deformed in its ground state minimum

point which is located at $\gamma = 0$ axis. Similarly, the PES of ^{28}Si shows that it has the oblate minimum energy along $\gamma = 60$ axis as can be seen in Fig. 2(c). From these figures, we can conclude that these nuclei are axially symmetric.

Summary and Future Work

In this work, we have calculated the energy surfaces as a function of deformation parameter for some light nuclei, namely, ^{16}O, ^{22}Ne and ^{28}Si. We also calculate the energy surfaces in $(\beta - \gamma)$ plane in order to check the deviation from axial symmetry in these nuclei. It is found that ^{16}O nucleus has spherical shape as it can be expected and the other two nuclei ^{22}Ne and ^{28}Si have prolate and oblate shapes, respectively. No deviation from axial symmetry is found for these two deformed nuclei.

Recent experiments suggest that nuclei can have permanent triaxial shape. This new discovery motivates us to investigate the internal structure properties of the nuclei. We will investigate the existence of triaxial shapes in light nuclei by calculating the PES in $(\beta - \gamma)$ plane.

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