INVESTIGATION OF TRIAXIALITY IN MEDIUM-MASS GERMANIUM ISOTOPES

Khaing Pwint Wai[1], Nyein Wint Lwin[2]

Abstract

The shape evolution for some selected germanium isotopes have been investigated from calculated potential energy surfaces on beta-gamma $(\beta-\gamma)$ plane and analyzed by the single-particle energy levels. The Ev8 program with a 3-dimensional Cartesian mesh which solves the Skyrme-Hartree-Fock+BCS problem is employed. From the $(\beta-\gamma)$ plane, these results are pointed out that ^{64}Ge is to be triaxial while both ^{68}Ge (oblate) and ^{78}Ge (prolate) have axially symmetric whereas ^{82}Ge gives the spherical nature. The calculated binding energies of all selected nuclei in this work fairly agree with experimental data.

Keywords: Skyrme Hartree-Fock + BCS method, $(\beta-\gamma)$ plane

Introduction

One of the major challenges in nuclear physics is to study the nuclear structure of neutron-rich nuclei far from the beta stability line. For that reason, many researchers are trying to find out the valuable observations either experimentally or theoretically. There are about 4000–7000 nuclei which are expected to be bound from several theoretical calculations but have not yet been discovered experimentally. At present, both experimental results and theoretical calculations concluded that most of the deformed nuclei have a quadrupole deformation of the prolate kind (cigar-like shape) that preserves to a great extent axial symmetry. Therefore, those regions of the nuclide chart showing deformation with axial symmetry or deformed triaxial distributions breaking axial symmetry are of great interest to deepen the understanding of the mechanisms underlying the appearance of deformation [Robledo, L. M., R. R. Guzman and P. Sarriguren, (2009)].

The microscopic models with effective interactions are widely used to investigate the properties of nuclei in stable and unstable regions. These can be divided into two different approaches; the shell model and self-consistent mean-field models. The shell model plays a main role for calculating the ground-state properties and excitations of nuclei with a mean-field description which is built from phenomenological single-particle basis wave functions such as the harmonic oscillator. However, it cannot explain some observed parities of heavier excited nuclei and magnetic moments. In the past decades, the relativistic and non-relativistic self-consistent mean-field approaches have been popular to study the structures of nuclei. The self-consistent mean-field (SCMF) theory is the only approach that aims closer to a fully microscopic description of nuclei that is computationally tractable over the entire mass table, it becomes the successful approach to describe and predict the properties of heavy nuclei. Many of these nuclei are located in the neutron-rich region and they play an important role in explaining the nucleosynthesis mechanism beyond iron. Therefore, it is necessary to gain knowledge of the structures of neutron-rich nuclei which are quite different from that of stable nuclei.

The aim of this present work is to predict the shapes of medium-mass nuclei with quadrupole deformation using self-consistent mean field approach. In this work, we chose four germanium isotopes (^{64}Ge, ^{68}Ge, ^{78}Ge, ^{82}Ge) because they can exhibit a pronounced competition between different configurations. The structures of these nuclei will be investigated by calculating the potential energy surfaces on $(\beta-\gamma)$ plane which can clearly show the shapes of nuclei. To

[1] Assistant Lecturer, Department of Physics, Monywa University.
[2] Professor, Department of Physics, University of Mandalay.

this end, the Ev8 program will be employed in this work [Ryssens, W. et al, 2014]. This report is organized as: firstly, background theory of spherical shell model and deformed shell model will be discussed. Then Hartree-Fock equations with Skyrme interaction are presented. In addition constrained-Hartree-Fock method is also discussed. Finally, we concluded the results with the descriptions of the shapes which are obtained from the calculated potential energy surfaces.

Formalism

I. Background Theory of Spherical and Deformed Shell Model

The shell model which is based on the Schrödinger equations for the single-particle levels can be seen as follows

$$\left(-\frac{h^2}{2m}\nabla^2+V(\mathbf{r})\right)\psi_i(\mathbf{r})=\varepsilon_i\psi_i(\mathbf{r}) \tag{1}$$

where the central potential V(r) will be approximated by the phenomenological potential such as square well, the Woods-Saxon or harmonic oscillator potential. It was realized, however, that use of such a phenomenological potential alone cannot even reproduce the empirical shell closures without the inclusion of a spin-orbit coupling term, as shown by Mayer

$$H=-\frac{h^2}{2m}\nabla^2+V(\mathbf{r})+V_{so}(\mathbf{r})\hat{\ell}.\hat{s} \tag{2}$$

where $\hat{s}$ and $\hat{\ell}$ are spin and angular momentum operators for a single nucleon. The degeneracy of oscillator level was partially removed with the introduction of this $\hat{\ell}.\hat{s}$ term and the levels split up as $j=\ell\pm1/2$, where j is the total angular momentum.

Since the potential for the shell model was spherically symmetric so that a new potential was needed for deformed nuclei. The Nilsson model, modified shell model, has been one of the most successful models that ever developed in nuclear theory. The modified harmonic-oscillator potential introduced by Nilsson et al., has been extensively employed in the interpolation of deformed nuclei [Zhang, J.Y. et al.,1989]. For axially symmetric deformed shapes, the potential extension along the nuclear z-axis is different from the two equal frequencies in the x and y-axes. The single-particle Hamiltonian in the form as follows

$$H_{nil}=-\frac{h^2}{2M}\nabla^2+\frac{M}{2}\left[\omega_\perp^2\left(x^2+y^2\right)+\omega_z^2z^2\right]-2k\hbar\omega_0\vec{\ell}.\vec{s}-\mu'\hbar\omega_0\left(\ell^2-\left\langle\ell^2\right\rangle_N\right) \tag{3}$$

where ω_0 is the oscillator frequency for the spherical case related to each of the three dimensions, κ controls the strength of the spin-orbit part of the potential, and μ controls the strength of the correction term. The correction term, $\left(\ell^2-\left\langle\ell^2\right\rangle_N\right)$ originally had the form of $\mu\ell^2$. It served the purpose of suppressing (repressing) the energy of the higher lying shells; however, it was noted that this shift was too large for large N quantum numbers [Gustafson C. et al., 1968].

For triaxial nuclear shapes, the Hamiltonian in term of anisotropic harmonic oscillator potential becomes

$$H_{nil}=-\frac{h^2}{2M}\nabla^2+\frac{M}{2}\left(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2\right)-2k\hbar\omega_0\vec{\ell}.\vec{s}-\mu'\hbar\omega_0\left(\ell^2-\left\langle\ell^2\right\rangle_N\right) \tag{4}$$

The triaxial shape associated with the harmonic oscillator potential can be seen as follows

$$V_{osc} = \frac{M}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right) \tag{5}$$

with $\omega_x \neq \omega_y \neq \omega_z$ and their relationships with the parameter (β) and the triaxiality angle (γ) are

$$\omega_x = \omega_0(\beta,\gamma)\left[1-\frac{2}{3}\beta\cos\left(\gamma+\frac{2\pi}{3}\right)\right] \tag{6}$$

$$\omega_y = \omega_0(\beta,\gamma)\left[1-\frac{2}{3}\beta\cos\left(\gamma-\frac{2\pi}{3}\right)\right] \tag{7}$$

$$\omega_z = \omega_0(\beta,\gamma)\left(1-\frac{2}{3}\beta\cos\gamma\right) \tag{8}$$

The parameter (β) specifies the degree of deformation and the parameter (γ) describes the departure from axial symmetry.

The deformation dependence of $\omega_0(\beta,\gamma)$ is determined from volume conservation of the ellipsoidal equipotential surfaces. For the static nuclei, it is needed only the one sector $0^\circ \le \gamma \le 60^\circ$. The nucleus is assumed to have prolate shape when $\gamma = 0^\circ$ and oblate shape for $\gamma = 60^\circ$ and the intermediate $\gamma-$values as the triaxial shape. The single-particle energies of the triaxial modified oscillator Hamiltonian are obtained from diagonalisation.

With these definitions and the Nilsson Hamiltonian, the energy eigen states $\left(\varepsilon_{K^\pi[Nn_z\Lambda]}\right)$, sometimes called Nilsson orbitals, can be extracted from solving the Schrödinger equation.

$$H_{nil}\psi_i = \psi_i\varepsilon_i \tag{9}$$

where i represents the complete set of asymptotic quantum numbers used to specify Nilsson orbitals

$$K^\pi\left[Nn_z\Lambda\right] \tag{10}$$

where *K* is the quantum number defines the overlap of the orbital with the deformed core, π is the parity defined as $\pi = (-1)^\ell = (-1)^N$, *N* is the oscillator quantum number, n_z is the number of oscillator quanta (number of nodes in the wave function), and Λ is the projection of the particle's orbital angular momentum onto the symmetry axis.

II. Hartree-Fock Equations with Skyrme Interaction

The full many-body Hamiltonian with a one-body kinetic energy term and a two-body force is obtained as follows

$$H = \sum_{i=1}^{N}\hat{t}_i + \frac{1}{2}\sum_{i\neq j}^{N}\hat{V}(r_i, r_j) \tag{11}$$

where the first term gives the kinetic energy operator and the second is the two-body force with the Coulomb interaction. Finally, the simplified expression for the Hatree-Fock equations becomes

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U_H^{(i)}(\mathbf{r})\right)\varphi_i(\mathbf{r}) - \int d\,\mathbf{r}' U_F^{(i)}(\mathbf{r},\mathbf{r}')\varphi_i(\mathbf{r}') = \varepsilon_i\varphi_i(\mathbf{r}). \tag{12}$$

This equation is known as the Hartree-Fock equation. The first term is known as the Hartree potential (the local term). The latter non-local part is also called the Fock term. In the following, the Skyrme approximation which can greatly reduce the number of integrations over single particle states will be discussed.

In the Skyrme-Hartree-Fock approach, the total binding energy of the system is given by the sum of the kinetic, Coulomb energies and the Skyrme energy functional that models the effective interaction between nucleons [Bender M. et al., 2003]. The full Skyrme interaction can be shown in the form of the following equation,

$$E = E_{Coulomb} + E_{kin} + E_{Sk} \ . \tag{13}$$

The result of the Hartree-Fock equations with Skyrme interaction is

$$\begin{aligned} E_{sk} &= b_1\rho^2 + b_2\left(\rho_n^2 + \rho_p^2\right) + b_3\tau\rho + b_4\left(\tau_n\rho_n + \tau_p\rho_p\right) + b_5\rho\nabla^2\rho \\ &+ b_6\left(\rho_n\nabla^2\rho_n + \rho_p\nabla^2\rho_p\right) + b_7\rho^{\alpha+2}(\mathbf{r}) + b_8\left(\rho_n^{\alpha+2} + \rho_p^{\alpha+2}\right) \\ &+ b_9\rho\vec{\nabla}J + b_{10}\left(\rho_p\vec{\nabla}J_p + \rho_n\vec{\nabla}J_n\right) + b_{14}J^2 + b_{15}\left(J_n^2 + J_p^2\right) \end{aligned} \tag{14}$$

In constrained Hartree-Fock (CHF) method, a wave function such as $\left|\Phi(q)\right\rangle$ is used to minimize the total energy under the constraint that a certain single-particle operator $\left\langle\hat{Q}\right\rangle$ which has a fixed expectation value

$$q = \left\langle \Phi \middle| \hat{Q} \middle| \Phi \right\rangle. \tag{15}$$

The method to solve this problem is adding to the Hamiltonian H in the condition Eq. (15) with Lagrange multiplier λ with quadrupole operators Q_{20} and Q_{22} which are constrained and can be seen as follows

$$\left\langle H' \right\rangle = \left\langle H \right\rangle - \lambda_1 \left\langle \hat{Q}_{20} \right\rangle - \lambda_2 \left\langle \hat{Q}_{22} \right\rangle. \tag{16}$$

In this work, this method is used to calculate the energy surface as a function of collective parameters of "q" such as quadrupole deformation.

Results and Discussion

In this calculation, the potential energy surfaces (PES) for selected even-even germanium isotopes are studied to investigate whether it has axially deformed or not. The axial deformation can give either prolate or oblate shape; on the other hand, the non-axial deformation leads to the triaxial shape. There are many sets of the Skyrme parameters. The Sly4 parameter set is chosen for this calculation because this parameterization can give good agreement for the nuclear root mean square radii and binding energies. The zero-range density dependence pairing force will be used in this calculation.

The relationship between the deformation parameter (q) and the triaxiality angle (γ) can be represented by

$$q_1 = q\cos(\gamma) - \frac{1}{\sqrt{3}}\, q\sin(\gamma) \tag{17}$$

$$q_2 = \frac{2}{\sqrt{3}}\, q\, \sin(\gamma). \tag{18}$$

The representation of deformation parameter $\beta_{\ell m}$ which is related to the total mass of the moment as follows

$$\beta_{\ell m} = \frac{4\pi}{3R_0^{\ell} A} \left\langle \hat{Q}_{\ell m} \right\rangle \tag{19}$$

In this section, the calculated potential energy curves using constrained Hartree-Fock method are depicted in Fig. 1 for four selected germanium nuclei (^{64}Ge, ^{68}Ge, ^{78}Ge and ^{82}Ge).

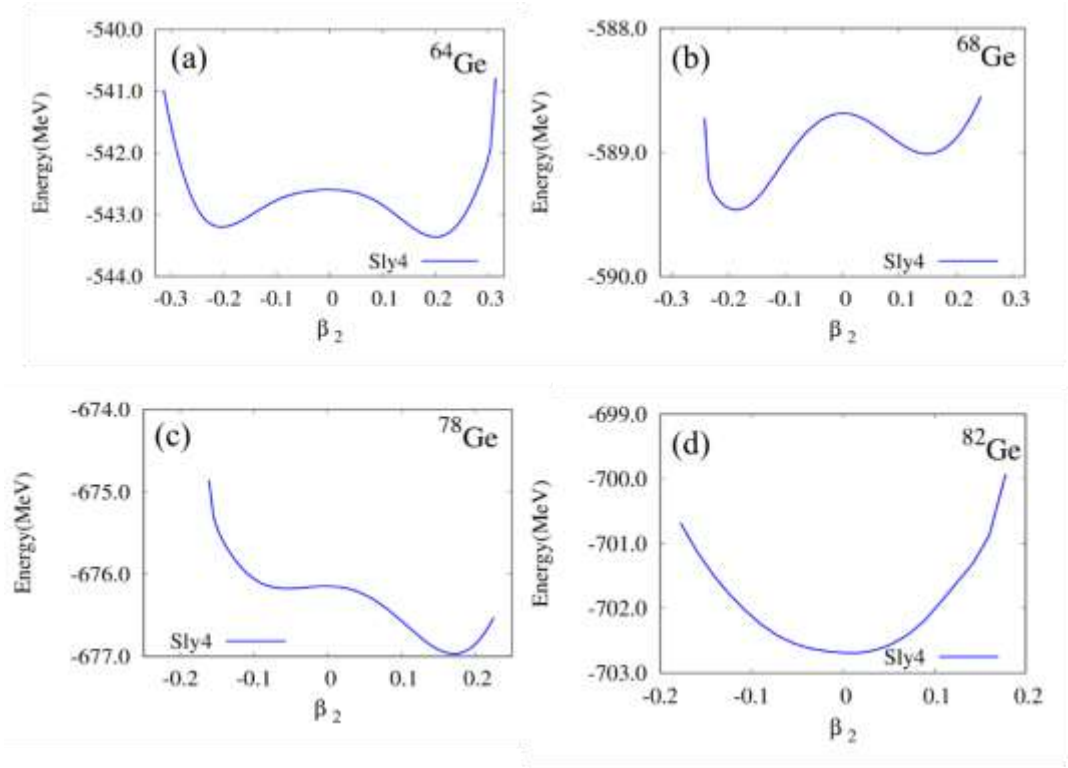

Figure 1 The potential energy curve versus quadruple deformation (β_2) for (a) ^{64}Ge, (b) ^{68}Ge, (c) ^{78}Ge and (d) ^{82}Ge nuclei obtained with the Sly4 parameter set.

In this section, we first calculate the potential energy surfaces as a function of axial quadrupole deformation parameter. The calculated potential energy surfaces are depicted in Fig. 1(a-d) for ^{64}Ge, ^{68}Ge, ^{78}Ge and ^{82}Ge nuclei. The nuclei having minimum energy located at the positive deformation parameter generally describes the prolate shape while the minimum energy with negative deformation parameter stands for the oblate shape. The ground state energy located at the origin is predicted to have the spherical shape. The shape coexistence is expected in ^{64}Ge nucleus since the energy difference between oblate and prolate shape is less than 0.3 MeV. Shape evolution has been found from oblate to prolate and spherical in ^{68}Ge, ^{78}Ge and ^{82}Ge nuclei. The ^{68}Ge nucleus is predicted to have minimum oblate configuration which can be seen in panel (b) whereas ^{78}Ge to be prolate sides in panel (c), respectively. The semi-magic ^{82}Ge nucleus shows the spherical shape in the last panel (d).

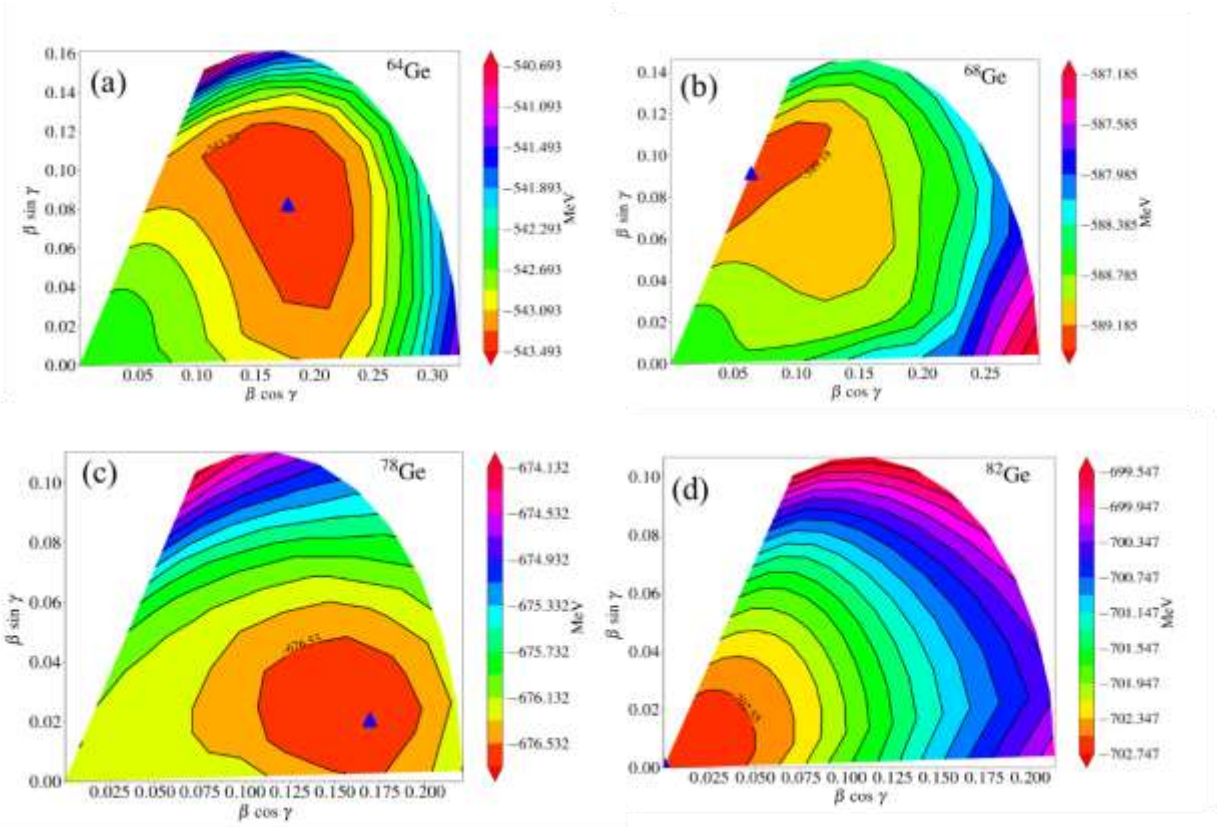

Figure 2 The potential energy surfaces versus quadruple deformation (β_2) for (a) ^{64}Ge, (b) ^{68}Ge, (c) ^{78}Ge and (d) ^{82}Ge nuclei on $\beta-\gamma$ plane obtained with Sly4 parameter set.

In order to investigate whether there is a deviation from axial symmetry in these nuclei, it is necessary to calculate the potential energy surfaces on $\beta-\gamma$ plane (See: Fig. 2(a)-(d)).In above figures, the contours join the points with the same energy and each contour line is separated by 0.2 MeV. The triangles in these figures indicate the absolute minimum in the potential energy surfaces.

As can be seen in Fig. 2(a), the PES for ^{64}Ge shows its minimum energy at points which is deviating from axial symmetry (ie., the energy minimum does not occur at either $\gamma=0°$ or $\gamma=60°$). This fact suggests that this nucleus is expected to have triaxial nature. It has ground state energy of 543.29 MeV at $\beta_2\approx0.18$ and triaxiality angle $\gamma=25^{\circ}$.The PES of ^{68}Ge shows oblate minimum which is located at $\beta_2\approx0.11$ on $\gamma=60°$ axis having 589.18 MeV as shown in panel (b). On the contrary, the calculated results suggest that ^{78}Ge nucleus can have more prolately deformed configuration rather than the soft-triaxial nature giving ground state energy of 676.53 MeV with the quadrupole deformation nearly 0.17 (See: Fig. 2(c)). Finally, the potential energy surface (PES) for the semi-magic number ^{82}Ge nucleus is showing spherical configuration at the origin with minimum energy of 702.55 MeV.

The variation of single particle energy levels as a function of quadrupole deformation will be discussed in the next section.

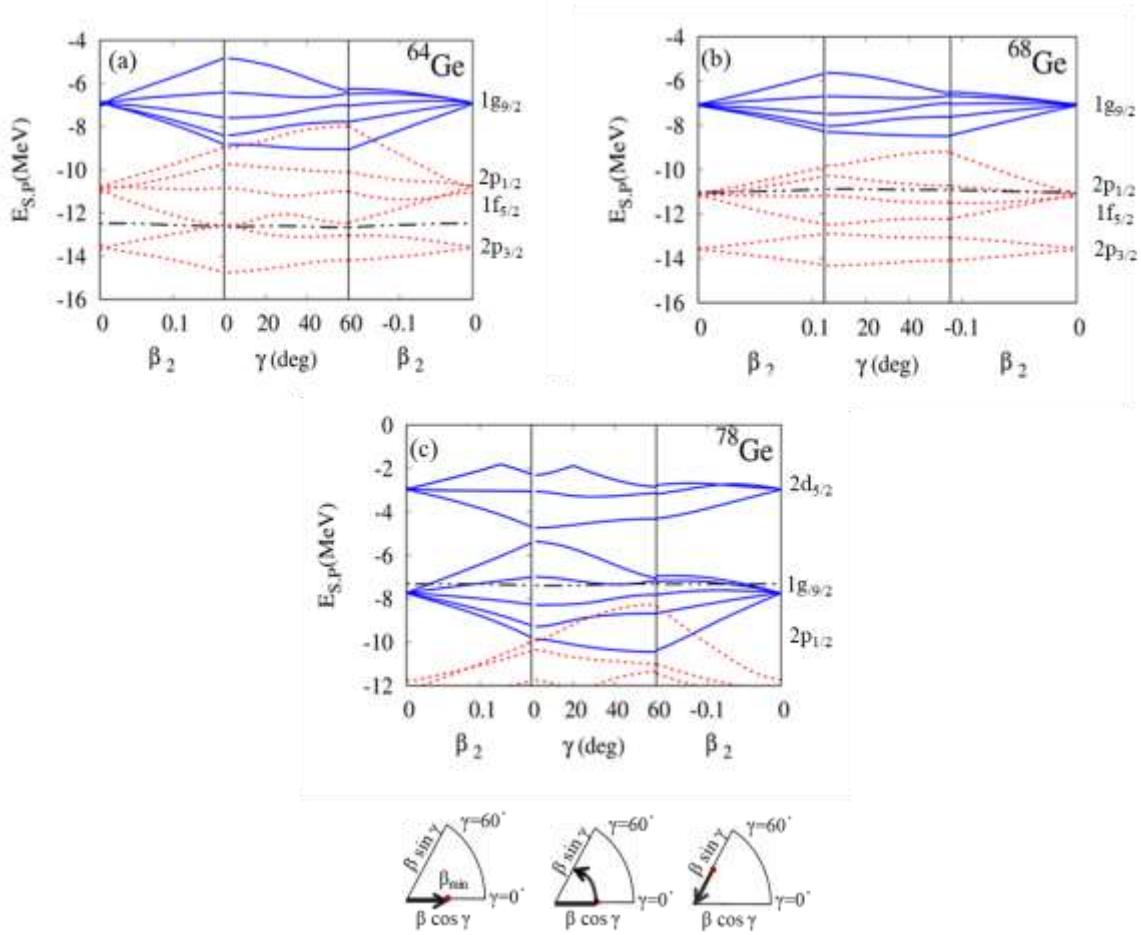

Figure 3 Schematic diagrams for single-particle orbitals along a path (β, γ) are depicted in the lower part of the figures. Combined plot of neutron single-particle energies (a) ^{64}Ge, (b) ^{68}Ge and (c) ^{78}Ge nuclei plotted as a function of the deformation parameter.

In order to get more inside on the resultant nuclear configurations, the single particle levels as a function of triaxial degrees of freedom is plotted in Fig. 3(a-c). It is known that the formation of deformed minima is favored by the occurrence of gaps or low single-particle level density around the highest occupied level. In these figures, the neutron SPE for each selected nuclei are depicted as the combined plot. In the combined plot, the axially symmetric single-particle levels are plotted as a function of deformation parameter (β_2) on the left and right-most panels. In the middle panel, neutron levels are plotted as functions of γ-deformation parameter for a fixed value (β_2) which corresponds to the ground state minimum. Solid blue curves with positive parity, short-dotted red curves with negative parity, and dashed black curve corresponds to the Fermi level and red circles indicated the magic number. Figure 3 (a) is for ^{64}Ge. In this figure, a pronounced gap appears near the Fermi Level which is found between the last occupied $2p_{3/2}$ and first unoccupied states $1f_{7/2}$ sub-shell. The appearance of gap in the triaxial region, $20^{\circ} < \gamma < 30^{\circ}$, favors the triaxial shape. The appreciable gap on the oblate axis near the Fermi level is found for ^{68}Ge nucleus which is shown in panel (b). Meanwhile, ^{78}Ge nucleus has the formation of the oblate and prolate neutron gaps which are found above the Fermi level but the largest gap is found on the prolate axis which favours the deep prolate configuration as can be seen in panel (c).

Summary and Conclusion

In this research work, we first calculate the potential energy curves as a function of quadrupole deformation parameter for four even-even germanium isotopes using the Sly4 parameter set. The results suggest that start from shape coexistence in ^{64}Ge nucleus, the shape evolution, ie., oblate-prolate-spherical shapes is found in ^{68}Ge, ^{78}Ge and semi-magic nucleus, ^{82}Ge.

In order to determine the existence of axial asymmetry in these nuclei, the potential energy surfaces of these nuclei are calculated on $\beta-\gamma$ plane. These results confirm oblate, prolate and spherical shapes for ^{68}Ge, ^{78}Ge and ^{82}Ge nucleus, respectively. On the contrary, the energy minimum of ^{64}Ge occurs at $\gamma = 25^{\circ}$,ie., triaxial shape.

Finally the single-particle energies on $\beta-\gamma$ plane for three deformed germanium nuclei are computed to examine the shapes of nuclei. It can also be concluded that the preference of ground state shape configurations is sensitive on the slope of last occupied single particle level.

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