

Calculation of the total potential between two deformed heavy ion nuclei using the Monte Carlo method and M3Y nucleon-nucleon forces

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In the current study, a simulation technique has been employed to calculate the total potential between two deformed nuclei. It has been shown that this simulation technique is an efficient one for calculating the total potential for all possible orientations between the symmetry axes of the interacting nuclei using the realistic nuclear matter density and the M3Y nucleon-nucleon effective forces. The analysis of the results obtained for the $^{48}\text{Ca} + ^{238}\text{U}$, $^{46}\text{Ti} + ^{46}\text{Ti}$, and $^{27}\text{Al} + ^{70}\text{Ge}$ reactions reveal that considering the density dependent effects in the M3Y forces causes the nuclear potential to drop by an amount of 0.4 MeV.

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I. INTRODUCTION

Since the interaction between two deformed nuclei could be a way to access the proposed islands of superheavy nuclei, the calculation of the nucleus-nucleus potential between two deformed, oriented nuclei is one of the main subjects that has attracted great interest in theoretical heavy ion physics [1–8]. Recent studies on the interactions between deformed nuclei using the double folding (DF) formalism reveal that the physically significant region of the HI potential is strongly associated with the orientation of the symmetry axes of the participant nuclei [2,6,7]. Therefore, the amount of overlapping of the nuclear density in these regions depends on the different orientations of the symmetry axes of the two nuclei participating in the reaction. This and the fact that nucleon-nucleon (NN) interaction forces are of M3Y kind that depends on the density have motivated us to conduct this study to find out to what extent the density dependent terms in the M3Y interaction affect the calculation of the total potential in the reactions of the deformed nuclei. Since we are going to study the effect of this correction on the calculation of the total potential, we have, therefore, ignored the effects such as channel coupling and the possibility of the exchange of neutrons between the projectile and the target nuclei during the fusion process.

In order to calculate the total potential between deformed nuclei using the M3Y NN forces, one has to employ a suitable formalism such as the DF model [9]. However, the calculations of the DF formalism for two deformed nuclei lead to a six-dimensional integral that makes the task of its precise evaluation formidable. Among different methods suggested to simplify the calculation of the six-dimensional integral of the DF model, the multipole expansion for the nuclear density distribution function is a suitable method for the evaluation of the total potential in the interaction between deformed nuclei [10]. In this method the use of the Fourier transform of the total potential and the multipole expansion of the nuclear density distribution function reduce the six-dimensional integral of the DF model to a sum of the products

of the three single dimensional integrals. However, taking into account the corrections due to the density dependent effects in the M3Y NN interactions greatly complicates the analytical calculations of this formalism. Thus, in the investigations of the heavy-ion interactions, it is usually advantageous to seek methods that can accurately and quickly calculate the total potential using two deformed density distributions that take into account the density dependent effects in the interactions of nucleons for all possible orientations of symmetry axes of nuclei participated in the reaction. To this end, we have extended the simulation method previously that we used to calculate the total potential in the interaction of the two heavy-ion spherical nuclei [11], to the calculation of the total potential of deformed nuclei.

In Secs. II and III we shall briefly discuss the calculations of the DF model using the multipole expansion of the nuclear matter density and the Monte Carlo methods, respectively. Comparison between the results of the multipole expansion and the Monte Carlo methods is given in Sec. IV. In Sec. V we discuss the effect of the density dependent terms in the M3Y NN interaction on the calculation of the total potential. Section VI is devoted to some concluding remarks.

II. THE DF MODEL AND THE MULTIPOLE EXPANSION OF THE NUCLEAR DENSITY

In general the calculation of the total potential plays a key role in the investigation of interactions between deformed nuclei. One of the models commonly used to calculate this potential is the DF model. If the orientation of the symmetry axes of the nuclei participating in the reactions with respect to the fixed laboratory frame is denoted by a set of Euler angles Ω_i for each nucleus, then using the effective nucleon-nucleon potential $V_{NN}(s)$, and the internuclear potential is given by

$$V(R, \hat{\Omega}_P, \hat{\Omega}_T) = \int \rho_P(\mathbf{r}_1, \hat{\Omega}_P) \rho_T(\mathbf{r}_2, \hat{\Omega}_T) V_{NN}(s) d\mathbf{r}_1 d\mathbf{r}_2, \quad (1)$$

where $\mathbf{s} = \mathbf{R} + \mathbf{r}_2 - \mathbf{r}_1$. The coordinate system for the interacting deformed-deformed nuclei is indicated in Fig. 1. Now if one uses the multipole expansion function of the nuclear

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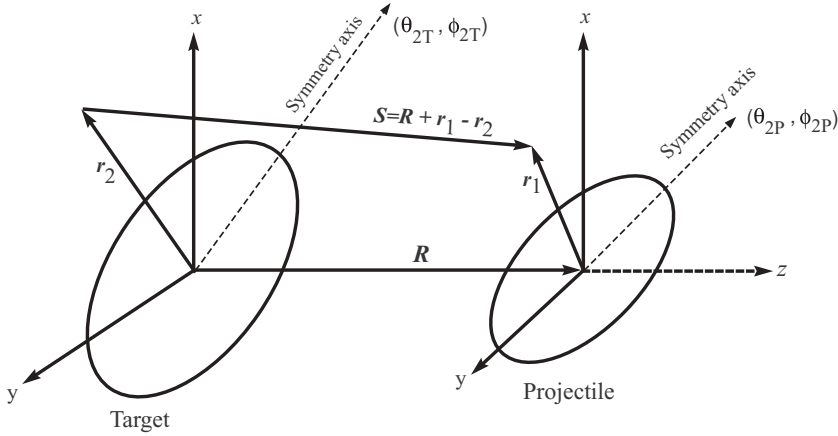


FIG. 1. Geometry of the collision between two deformed nuclei. (θ_{2P}, ϕ_{2P}) and (θ_{2T}, ϕ_{2T}) are the angles that the symmetry axes of the projectile and the target nuclei make with a fixed reference direction in space.

density functions along with the Euler matrices in order to relate the nuclear density in body-fixed frame to that in the lab-fixed frame, in the calculations of the DF model we can get [2,10]

$$\begin{aligned}
 V(R, \hat{\Omega}_P, \hat{\Omega}_T) &= (4\pi)^3 \sum_{\lambda_1 \lambda_2 \lambda} i^{\lambda_1 + \lambda - \lambda_2} (2\lambda + 1) \begin{pmatrix} \lambda & \lambda_1 & \lambda_2 \\ 0 & 0 & 0 \end{pmatrix} \\
 &\times \int dq q^2 j_\lambda(qR) V_{NN}(q) \tilde{C}_{\lambda_2}^T(q) \tilde{C}_{\lambda_1}^P(q) \\
 &\times \sum_{m=-\lambda_1}^{m=+\lambda_1} (-1)^m \begin{pmatrix} \lambda & \lambda_1 & \lambda_2 \\ 0 & m & -m \end{pmatrix} Y_{\lambda_1 m}^*(\hat{\Omega}_P) Y_{\lambda_2 m}(\hat{\Omega}_T), \quad (2)
 \end{aligned}$$

where

$$V_{NN}(q) = \frac{1}{(2\pi)^3} \int d\mathbf{x} e^{-i\mathbf{q}\cdot\mathbf{x}} V_{NN}(\mathbf{x}), \quad (3)$$

$$C_\lambda(r) = \int d\Omega_{\hat{\mathbf{r}}} \rho(\mathbf{r}) Y_{\lambda,0}(\hat{\mathbf{r}}), \quad (4)$$

$$\tilde{C}_\lambda(q) = \int dr r^2 C_\lambda(r) j_\lambda(qr). \quad (5)$$

Here $C_\lambda(r)$ is in fact the radius dependent function in the multipole expansion of nuclear density, i.e., $\rho_i(\mathbf{r}) = \sum_\lambda C_\lambda(r) Y_{\lambda,0}(\hat{\mathbf{r}})$. In these calculations the density distribution functions of the deformed nuclei are assumed to be of the form of the Fermi distribution function,

$$\rho(\mathbf{r}) = \frac{\rho_0}{1 + e^{\frac{r - R(\hat{\mathbf{r}})}{a}}}, \quad (6)$$

where $R(\hat{\mathbf{r}}) = R_0(1 + \sum_{l \geq 2} \beta_l Y_{l,0}(\hat{\mathbf{r}}))$ and β_l are the deformation coefficients of the nuclei.

III. THE SIMULATION METHOD

In our previous work, we purposed a Monte Carlo simulation technique for the calculation of the total potential in the interaction of the two heavy-ion spherical nuclei [11]. In this method, each of the participating nuclei in the reactions has been considered to be a bulk of randomly distributed points where each point represents the position of the constituent nucleons of the nuclei and their distribution obeys the nuclear density distribution.

In order to calculate the total potential of the deformed nuclei employing the proposed simulation technique one has to use the density function of the deformed nuclei instead of that of spherical nuclei. The density function of the deformed nuclei is assumed to be given by

$$\rho(r, \theta, \phi) = \frac{\rho_0}{1 + \exp[(r - R(\theta, \phi))/a]}, \quad (7)$$

where

$$R(\theta, \phi) = R_0 \left[1 + \sum_{l,m} \beta_{lm} Y_{l,m}(\theta, \phi) \right] \quad (8)$$

and β_l are the deformation parameters of the nucleus. For spherical nuclei these parameters are equal to zero. We have extended this relation for the nuclei that their axes of symmetry make angles θ_2 and ϕ_2 with a fixed direction in space. Using the addition theorem for spherical harmonics, we have

$$\begin{aligned}
 R(\theta_1, \phi_1; \theta_2, \phi_2) &= R_0 \left[1 + \sum_{l,m} \beta_l (-1)^l Y_{l,m}(\theta_1, \phi_1) Y_{l,-m}(\theta_2, \phi_2) \right] \quad (9)
 \end{aligned}$$

and the nuclear matter density of these nuclei is given by

$$\rho(r, \theta_1, \phi_1; \theta_2, \phi_2) = \frac{\rho_0}{1 + \exp[(r - R(\theta_1, \phi_1; \theta_2, \phi_2))/a]}, \quad (10)$$

where θ_1 and ϕ_1 are the angles between \mathbf{r} and a fixed direction in space. \mathbf{r} is a position vector at which the density is evaluated by Eq. (10) when the symmetry axis makes angles θ_2 and ϕ_2 with respect to the fixed direction in space. For the nuclei that have their symmetry axes rotated with respect to a fixed reference axis in space, the nuclear matter distribution is given by Eq. (10).

Random distribution of the nucleons inside a nucleus represents an unstable state of that nucleus. In order to simulate a true nucleus in its ground state, one has to randomly displace the nucleons in small distances in a way that the following two requirements are met. Firstly, the sum of the Coulomb and nuclear potentials between the nucleons agree with the experimental value of the binding energy of the nucleus in its ground state, and secondly, for the spherical nuclei the R_{rms} parameter should agree with its experimental value. For

TABLE I. The values of the quadruple (β_2), hexadecapole (β_4) deformation parameters, and R_0 , a_0 for the charge distribution. Values of these parameters are determined by HFB calculation [14].

Nuclei	β_2	β_4	R_0	a_0
^{48}Ca	0.0	0.0	3.8871	0.4673
^{238}U	0.24	0.02	7.0727	0.4496
^{46}Ti	0.24	0.01	3.9081	0.4804
^{27}Al	-0.33	-0.04	3.1595	0.4646
^{70}Ge	-0.24	-0.04	4.4741	0.5362

deformed nuclei we have substituted the R_{rms} parameter by the $\langle R_x^2 \rangle$, $\langle R_y^2 \rangle$, and $\langle R_z^2 \rangle$ parameters. The nucleon displacements are possible by both dynamic and static methods and in this paper we have used the latter. We have also used the BDM3Y1-Paris potential to calculate the nuclear potential between the nucleons inside the nucleus.

In order to calculate the total potential, we have calculated the sum of all interactions between the nucleons that constitute the target and the projectile nuclei. We have repeated these calculations for different arrangements of nucleons keeping the angles representing the symmetry axes of the deformed nuclei with respect to a reference axis in space fixed, until the average variations of the total potential become less than 0.1%.

In this proposed simulation method nucleons inside the nucleus are distributed randomly and their position is defined by the nuclear matter distribution function, so the value of the density of the nuclear matter in the site of the nucleons is known and we need not recalculate the nuclear density when we calculate the interaction between nucleons. Therefore, by employing our method of simulation, we can easily calculate the density dependent function in the NN interaction [see Eq. (13)]. It seems that our proposed method is a convenient method that can be used in the calculation of the total potential between the two deformed nuclei in the density dependent NN interaction.

IV. THE MONTE CARLO SIMULATION VS THE DF

In order to examine the possibility of using the purposed simulation method in the calculations of the total potential of the deformed heavy ion reactions, we have chosen the $^{48}\text{Ca} + ^{238}\text{U}$, $^{46}\text{Ti} + ^{46}\text{Ti}$, and $^{27}\text{Al} + ^{70}\text{Ge}$ reactions. At least, one of the participating nuclei in these reactions is considered to be deformed in its ground state. The total potential for these reactions using both the Monte Carlo simulation and the DF methods considering different orientations of the symmetry axes of the involved nuclei has been calculated and compared with each other.

In the calculations of the nucleus-nucleus potential for these reactions in both the DF model and the proposed simulation method, the nuclear matter densities of the target and the projectile nuclei for simplicity are assumed to be proportional to the charge densities in these nuclei (i.e., $\rho_A = \rho_Z A/Z$). In these calculations we have used the two parameter Fermi distribution (2PF) for proton densities. The parameters of density for the participant nuclei that are obtained from Hartree-Fock-Bogoliubov (HFB) calculations [14] are given in Table I.

The density independent effective NN interaction of the M3Y-Reid [12] type has been employed to calculate the nuclear potential. The direct part of this effective NN interaction is given by

$$v_{\text{dir}}(s) = v_{00}(s) + \frac{N_1 - Z_1}{A_1} \frac{N_1 - Z_1}{A_1} v_{01}(s). \quad (11)$$

To calculate the exchange term in the nuclear potential we have used the zero-range approximation,

$$v_{\text{ex}}(s) = \left(\hat{J}_{00} + \frac{N_1 - Z_1}{A_1} \frac{N_1 - Z_1}{A_1} \hat{J}_{01} \right) \delta(s), \quad (12)$$

where s is the distance between two nucleons. The explicit form of the expressions for v_{00} , v_{01} , \hat{J}_{00} , and \hat{J}_{01} are given, for example, in Ref. [13]. Since the ground state spin of one of the participating nuclei is zero in the chosen reactions, therefore the spin dependent terms of the M3Y interaction are relatively unimportant, thus we have not considered their

TABLE II. Comparison of the fusion barrier and its location calculated from the Monte Carlo simulation (MN) method with those obtained from the DF model. Calculation are made at different orientation angles (θ_T , ϕ_T) and (θ_P , ϕ_P) of the symmetry axes of the target and the projectile nuclei, respectively.

Reaction	Orientation angles (θ_T , ϕ_T) (θ_P , ϕ_P)	R_{DF} (fm) ^a	B_{DF} (MeV) ^a	R_{MN} (fm) ^b	B_{MN} (MeV) ^b
$^{48}\text{Ca} + ^{238}\text{U}$	(0,0) (0,0)	13.85	186.28	13.88	186.25
	(45,0) (0,0)	12.99	194.04	12.95	194.06
	(90,0) (0,0)	12.14	201.35	12.19	201.28
$^{46}\text{Ti} + ^{46}\text{Ti}$	(0,0) (0,0)	11.25	59.57	11.25	59.67
	(45,0) (0,0)	10.82	61.28	10.81	61.37
	(90,0) (0,0)	10.41	63.15	10.42	63.11
	(90,0) (90,0)	9.61	66.79	9.61	66.83
$^{27}\text{Al} + ^{70}\text{Ge}$	(45,0) (135,0)	9.82	56.09	9.80	56.12
	(45,45) (135,0)	9.86	55.95	9.88	55.97
	(45,90) (135,0)	9.92	55.58	9.93	55.66

^aThe values of the fusion barrier and its location obtained by the DF method.

^bThe values of the fusion barrier and its location obtained by the MN method.

effects in these calculations. Moreover, we neglect the possible energy dependence of these parameters.

Since the nuclear potential is of prime importance in the fusion cross-section calculations, we have compared our obtained results using the Monte Carlo method for the fusion barrier height and its location with those obtained using the DF method considering different orientations between the two symmetry axes of the interacting nuclei. The results are listed in Table II. It can be seen that the obtained results with both of these methods are in good agreement.

V. DENSITY-DEPENDENT NUCLEON-NUCLEON INTERACTION EFFECTS ON THE NUCLEUS-NUCLEUS POTENTIAL

It is known that the density dependence for effective the M3Y NN interaction is required to reproduce the basic properties of nuclear matter. In order to obtain the correct value of central nucleon density and nucleon binding energy, several versions of a density-dependent M3Y interaction have been proposed [15,16].

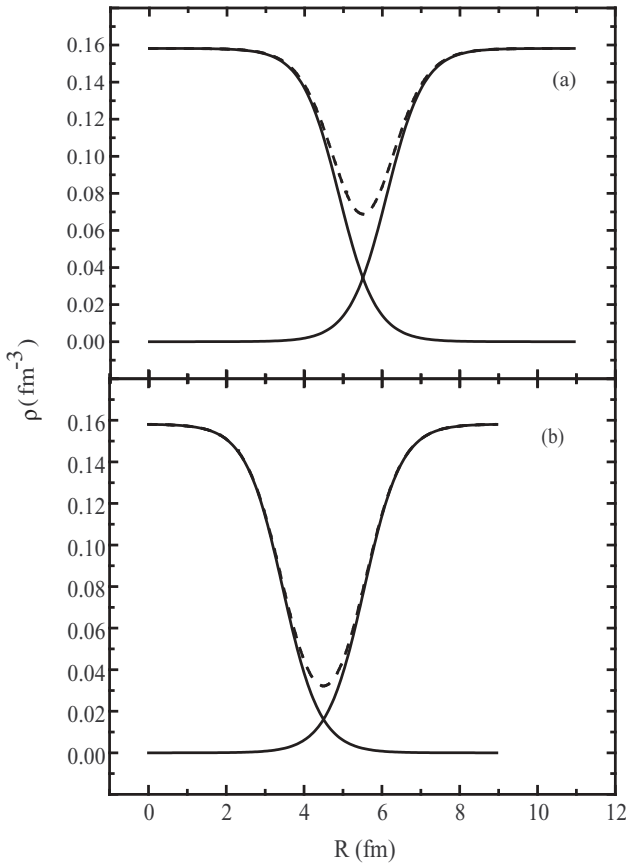


FIG. 2. The sum (dashed line) of the participant nuclei densities (solid lines) in the reaction $^{46}\text{Ti} + ^{46}\text{Ti}$ in the x-z plane for the orientations (a) (0,0)(0,0) and (b) (90,0)(90,0) are shown versus the distance between centers of two interacting nuclei. Densities of each nucleus have been calculated using Eq. (10) and to simplify these calculations the value of parameter θ_1 is assumed to be zero.

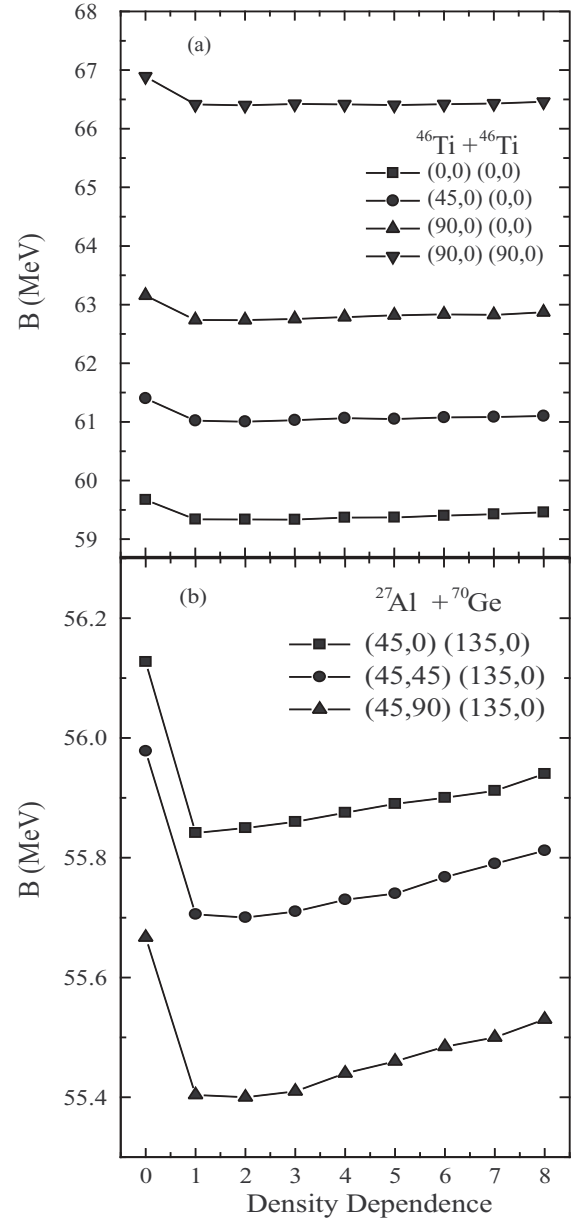


FIG. 3. The height of the fusion barrier for (a) $^{46}\text{Ti} + ^{46}\text{Ti}$ and (b) $^{27}\text{Al} + ^{70}\text{Ge}$ reactions have been calculated using several different versions of the density dependent M3Y interaction, the density dependence labels are listed in Table III. In this figure the orientation between target and projectile nuclei is indicated as $(\theta_{2T}, \phi_{2T})(\theta_{2P}, \phi_{2P})$.

The density dependence of the effective NN interaction of the M3Y type has been entered as a multiplier $f(\rho)$ in Eq. (11) where the function f is given by

$$f(\rho) = C(1 + \alpha \exp(-\beta\rho) - \gamma\rho), \quad (13)$$

the values of the C , α , β , and γ parameters for various interactions are given in Table III. For densities less than 0.11 fm^{-3} the density dependence leading to a stronger nuclear force since $f > 1$. The effect of this on the calculation of

TABLE III. The C, α , β , and γ parameters for several density dependent M3Y-Paris interaction [16].

DD label	Interaction	C	α	β (fm ⁻³)	γ (fm ⁻³)
0	D independent	1	0.0	0.0	0.0
1	DDM3Y1	0.2963	3.7231	3.7384	0.0
2	CDM3Y1	0.3429	3.0232	3.5512	0.5
3	CDM3Y2	0.3346	3.0357	3.0685	1.0
4	CDM3Y3	0.2985	3.4528	2.6388	1.5
5	CDM3Y4	0.3052	3.2998	2.3180	2.0
6	CDM3Y5	2.2728	3.7367	1.8294	3.0
7	CDM3Y6	0.2658	3.8033	1.4099	4.0
8	BDM3Y1	1.2521	0.0	0.0	1.7452

the total potential in the interaction between deformed nuclei depends on the amount of the overlap of the nuclear density due to different orientations of the axes of symmetry of the participant nuclei. For instance, Fig. 2 shows the total density variation in the $^{46}\text{Ti} + ^{46}\text{Ti}$ reaction for two different orientations of the symmetry axes of the participant nuclei. Here, the variation of the sum of the target and projectile nuclei densities is shown in the x-z plane as a function of distance between the centers of interacting nuclei. One can see that the variation of the overlap density for different angles of orientation is significant and this causes the density dependent function in the NN interaction to have different values. Therefore, the NN interaction will not have the same strength for different interaction angles.

In order to study this effect on the nucleus-nucleus potential we have calculated the height of the fusion barrier for the reactions $^{46}\text{Ti} + ^{46}\text{Ti}$ and $^{27}\text{Al} + ^{70}\text{Ge}$, using the method that we described in Sec. III. In these calculations the height of the fusion barrier has been calculated using several different versions of the density dependent M3Y interaction. Results are shown in Fig. 3. The obtained results for $^{46}\text{Ti} + ^{46}\text{Ti}$, Fig. 3(a), which are made at different polar angles show that accounting

for the density dependent decreases the height of the fusion barrier. It is clear from Fig. 3(b) that the calculation of the total potential depends on the azimuthal angle and accounting for density dependent effects will also decrease the height of the fusion barrier.

VI. CONCLUSION

In this paper we have employed a simulation technique based on the Monte Carlo simulation method for the calculation of the total potential between two deformed nuclei. The results obtained for the fusion barrier in the $^{46}\text{Ti} + ^{46}\text{Ti}$ and $^{27}\text{Al} + ^{70}\text{Ge}$ reactions (Table II) are in good agreement with those obtained by using the DF method. Therefore, by using this Monte Carlo simulation one can accurately calculate the total potential in the interactions between spherical-deformed and deformed-deformed nuclei. The simulation technique employed here has the ability of calculating the total potential taking into account the realistic nuclear matter density, all the possible deformation degrees of freedom, different orientations of the symmetry axes of the target, and the projectile nuclei with respect to each other and accounting the density dependent effect in the NN interactions.

We have also investigated the density dependent effects of the M3Y interaction on the calculation of the fusion barrier height, which is a physically important quantity in the field of heavy ion collisions. The obtained results reveal that the variation of fusion barrier height due to this effect depends on both the variation of the polar and azimuthal angles of the symmetry axis of the participant nuclei (Fig. 3).

The results obtained by the analysis of the $^{46}\text{Ti} + ^{46}\text{Ti}$ and $^{27}\text{Al} + ^{70}\text{Ge}$ reactions using the density dependent corrections in the M3Y forces show a decrease of about 0.4 MeV of the fusion barrier height in comparison to the corresponding values that are obtained using the density independent M3Y interaction.

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