Accuracy of multipole expansion of density distribution in calculating the potential for deformed spherical interacting pair

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The interaction potential for a deformed-spherical pair is calculated, and the error in using the truncated multipole expansion is evaluated for different numbers of terms of the expansion considered. It was found for the internal region of the nuclear part that three terms are sufficient, but for the surface and tail region up to five terms are necessary, while for the Coulomb potential three terms were found to be sufficient.

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In recent years, nuclear reactions involving deformed nuclei have become an important topic of research in nuclear physics [1]. One type of these reactions is the fusion reaction, which is an important intermediate step in the production of superheavy nuclei by heavy ion collisions. The nuclear potential between the interacting nuclei plays an important role in describing the reaction process.

A model that is commonly used in deriving a heavy ion (HI) potential is the double folding model [2]. The basic input into the folding calculation is the nuclear densities of the colliding nuclei. If one or both have deformed density distribution, the use of this model to derive Coulomb or nuclear interaction potentials becomes very difficult, since the six-dimensional integral cannot be simplified to fewer dimensions. In this case, one usually simplifies the folding model by expanding the density distribution of the deformed nuclei using a multipole expansion [3]. This method is useful and reduces the amount of calculation except in some cases, where the nucleon-nucleon (*NN*) force is density dependent. In the multipole expansion one may take a finite number of terms (usually three terms) and neglect the others [3]. Since this method is used frequently in deriving the real part of the HI potential for deformed-deformed and spherical-deformed pairs of nuclei, it is interesting to test its accuracy. In the present paper, we estimate the accuracy of the multipole expansion in deriving the heavy ion potential. We include both quadrupole and hexadecapole deformation parameters, and determine the number of terms in the multipole expansion needed to guarantee a very small percentage error.

We limit ourselves here to the interaction potential between deformed target and spherical projectile (see Fig. 1). The HI potential in this model is divided into a direct part U_d, and an exchange part $U_{\rm ex}$,

$$U(R,\beta)=U_d(R,\beta)+U_{\rm ex}(R,\beta). \quad (1)$$

They are stated in Refs. [2] and [3] as follows:

$$U_d(R,\beta)=\int d\mathbf{r}_1 d\mathbf{r}_2 \rho_T(\mathbf{r}_1) V_d(\mathbf{s}) \rho_p(\mathbf{r}_2), \quad (2)$$

$$U_{\rm ex}(R,\beta)=\int d\mathbf{r}_1 d\mathbf{r}_2 \rho_T(\mathbf{r}_1,\mathbf{r}_1+\mathbf{s}) V_{\rm ex}(\mathbf{s}) \rho_p(\mathbf{r}_2,\mathbf{r}_2-\mathbf{s}) e^{i\mathbf{k}\cdot\mathbf{s}/M}, \quad (3)$$

where R is the separation distance between the interacting nuclei, and β is the relative orientation angle of the target nucleus symmetry axis measured with respect to the separation vector $\mathbf{R}$.

The deformed density $\rho_T(r,\theta)$ has the form

$$\rho_T(r,\theta)=\frac{\rho_0}{1+e^{(r-R(\theta))/a}}, \quad (4)$$

where $R(\theta)$ is the half density radius expressed by the relation

$$R(\theta)=R_o[1+\delta_2 Y_{20}(\theta)+\delta_4 Y_{40}(\theta)]. \quad (5)$$

δ_2 and δ_4 are the quadrupole and hexadecapole deformation parameters.

The multipole expansion of the target nuclear density distribution has the form

$$\rho_T(\mathbf{r})=\sum_{lm} \rho_{lm}(r) Y_{lm}(\theta,\phi), \quad (6)$$

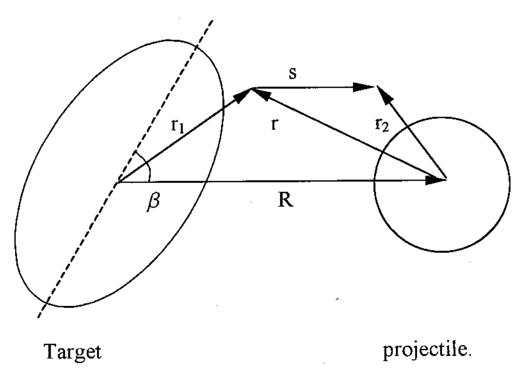

FIG. 1. The coordinate system.

and for an axially symmetric shape and limit the deformation to quadrupole and hexadecapole cases only, Eq. (6) is reduced to [4]

$$\rho(r,\theta)=\sum_{l=even}\rho_l(r)Y_{l0}(\theta), \tag{7}$$

the sum is usually truncated at $l=4$. Since the multipole expansion of the deformed nuclear or charge distribution is frequently used [3] to approximate the density form in Eq. (4), one should estimate the error in using the truncated expansion, Eq. (7). This error depends on the number of terms included in the expansion together with the order of deformation considered. For example, if only the quadrupole deformation is present, we get good accuracy using a small number of terms in the expansion, Eq. (7), while the existence of the quadrupole and hexadecapole deformations needs larger numbers of terms to have good representation of the deformed density, Eq. (4). The error in using multipole expansion depends also on the orientation angle of the deformed nucleus, and on the range of the *NN* force.

The aim of the present work is to estimate this error in calculating the direct part of the HI potential, since the calculation of the exchange part [5] for the deformed-spherical or deformed-deformed interaction pairs does not depend on the multipole expansion approximation. To calculate $U_d(R,\beta)$ for a deformed spherical nuclear pair, we start by transforming the integration variables in Eq. (2) defined by the relations

$$\mathbf{r}=\mathbf{r}_1-\mathbf{R}=\mathbf{r}_2-\mathbf{s},$$

which leads to

$$U_d(R,\beta)=\int d\mathbf{s}V_d(\mathbf{s})\int d\mathbf{r}\rho_T(\mathbf{R}+\mathbf{r})\rho_p(\mathbf{r}+\mathbf{s}), \tag{8}$$

where $\mathbf{s}$ is the vector joining the interacting nucleons.

Taking the Fourier transform of $\rho_p(\mathbf{r}+\mathbf{s})$, and noting that the projectile nucleus is spherical, the integration over $\mathbf{r}$ in Eq. (8) becomes

$$G^d(R,s,\beta)=8\int \rho_T(\mathbf{r}+\mathbf{R})\rho_p(x)\times j_o(kr)j_o(ks)j_o(kx)d\mathbf{r}k^2dkx^2dx.$$

Substituting in Eq. (8), one gets

$$U_d(R,\beta)=8\int k^2dk\int d\mathbf{r}\rho_T(\mathbf{r}+\mathbf{R})\times j_o(kr)\int d\mathbf{s}V_d(s)j_o(ks)\times\int j_o(kx)\rho_p(x)x^2dx. \tag{9}$$

The integration over $\mathbf{s}$ can be performed analytically for Coulomb, Yukawa, and Gaussian shapes of $V_d(s)$. Moreover, if the projectile nuclear density has a Gaussian or oscillator model shape, the integration over x can be performed. It should be noted that the above method of calculating U_d can be extended easily for density dependent finite range *NN* force.

To examine the accuracy of the multipole expansion of the matter or charge density distribution of a deformed target nucleus, one estimates the error in using this expansion in deriving the interaction potential for a deformed-spherical nuclear pair, such as the ^{238}U-^{16}O nuclear pair, for example. Figure 2 shows the percentage of error in the multipole density expansion against the radial distance r for two different values of the angle β=0.0°, 90.0°, and the deformation parameters of ^{238}U is taken to be $\delta_2=0.261$ and $\delta_4=0.0$, ± 0.087.

The percentage of error of the density

$$x_m=\frac{\rho_T-\rho_T^m}{\rho_T}\times 100\%, \tag{10}$$

where $\rho_T(r,\theta)$, is given by Eq. (4) and m is the upper sum limit in Eq. (7).

In Fig. 2(a), the error x_4 results from three terms in the multipole expansion for the values of r less than the deformed nucleus half radius (≈6.8 fm); the error in the expansion is negligible. For larger values of r, even for $\delta_4=0$, three terms of the multipole expansion are not sufficient to represent $\rho_T(r,\theta)$. The percentage of error x_4 (for $r>8.5$ fm and β=90°) reaches 20%, while for $\delta_4=+0.087$, it jumps to more than 80%. Figure 2(b) shows that four terms of the multipole expansion are sufficient for the case of $\delta_4=0.0$, β=0.0°, 90.0°, while Fig. 2(c) shows that five terms of the expansion reduce the errors in the two cases of $\delta_4=\pm 0.087$.

To show the effect of this error in calculating the Coulomb and nuclear potentials in a ^{238}U-^{16}O nuclear pair, we compare the calculated $U_d(R,\beta)$ using Eq. (9) with that based on a multipole expansion truncated after three, four, and five terms. We denote the latter by $U_d^m(R,\beta)$ for $m=4$, 6, and 8, and the method of calculating U_d^m is outlined in Ref. [3].

The *NN* potential used is the M3Y-Reid type, whose direct part consists of the two finite range interactions

$$V_d(s)=V_1+V_2,$$

where

$$V_1=7999\frac{e^{-4s}}{4s}, \tag{11a}$$

and

$$V_2=-2134.3\frac{e^{-2.5s}}{2.5s}. \tag{11b}$$

The zero range interaction is usually taken as an approximation for the finite range exchange part of the M3Y-*NN* potential, and is taken to be

$$V_{ex}(s)=V_3=-276\delta(\mathbf{s}). \tag{11c}$$

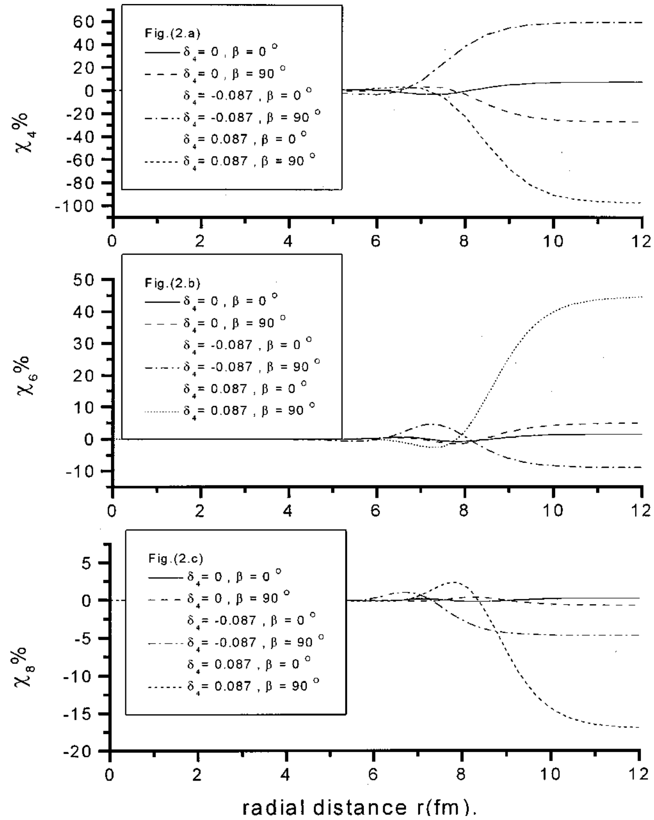

FIG. 2. The percentage of error in the multipole density expansion against the radial distance r for two different values of the angle β=0.0°, 90.0°.

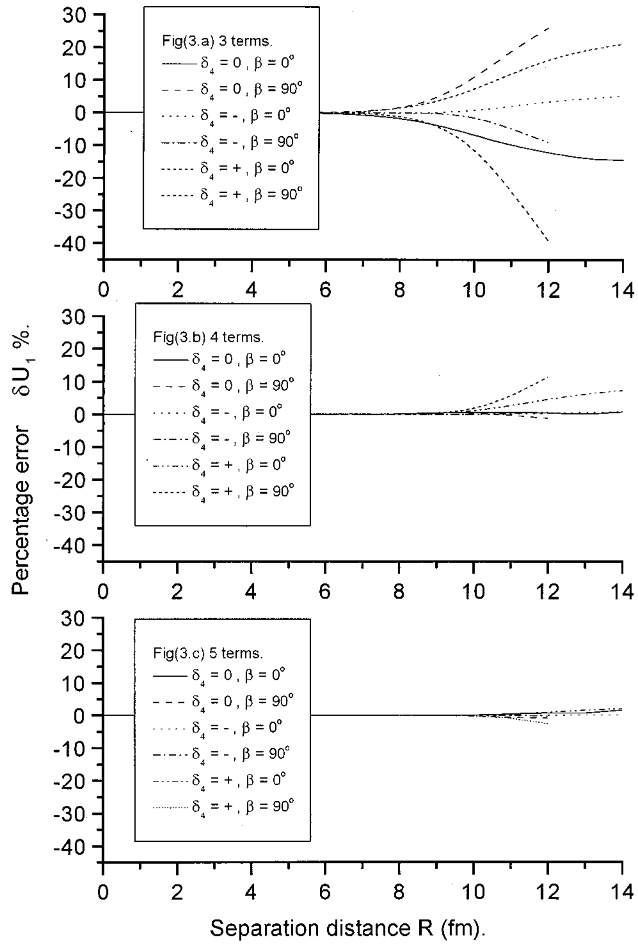

FIG. 3. Percentage of errors in folded potential δU_1^m.

Table I presents the percentage of error in the nuclear potential components for selected separation distances at the orientation angles β=0.0°, 90.0°, for a specific δ_4=0.087.

Figures 3–5 show the percentage of errors in the folded potentials δU_1^m, δU_2^m, and δU_3^m, based on the *NN* potentials V_1, V_2, and V_3, respectively, for all sets of parameters β, δ_2, and δ_4.

The results of the calculations can be summarized as follows:

(i) For Coulomb interaction, the error in using three terms in the multipole expansion was negligible for the three values of δ_4, and for the two orientation angles β=0.0, 90.0° of ^{238}U. Then the use of a multipole expansion with three terms is sufficient to calculate the Coulomb potential of the ^{238}U-^{16}O nuclear pair.

(ii) For the separation distance $R \leqslant 8$ fm the multipole expansion with only three terms can be considered enough for deriving the nuclear HI potential for the three values of δ_4. As the separation distance increases further, $|\delta U_i^4|$ increases also and becomes dependent on the range of *NN* force, the orientation angle, and the value of the hexadecapole deformation. The figures and the table show that three terms of the multipole expansion produce large errors in calculating the HI nuclear potential; it is more than 40% at R = 12 fm, β=90.0°, and δ_4=0.087, but for δ_4=0, this error is reduced to less than 20%.

TABLE I. Percentage of error in nuclear potential components for selected separation distances.

β^o	% error R (fm)	δU_1^4	δU_1^6	δU_1^8	δU_2^3	δU_2^4	δU_2^5	δU_3^3	δU_3^4	δU_3^5
0	8	1.545	0.128	0.002	1.473	0.118	−0.002	1.594	0.138	0.006
	10	7.363	1.115	0.015	6.741	1.000	0.017	7.843	1.207	0.010
	12	16.208	4.604	0.926	14.796	3.994	0.761	17.162	5.033	1.073
	14	21.250	7.292	2.83	19.937	6.593	1.727	21.918	8.219	2.740
90	8	−1.208	0.088	−0.012	−1.1116	0.083	−0.011	−1.268	0.099	−0.009
	10	−11.412	1.925	−0.128	−3.655	1.575	−0.106	−12.865	2.266	−0.146
	12	−39.114	11.439	−2.583	−32.785	9.216	−1.926	−42.693	13.415	−2.439

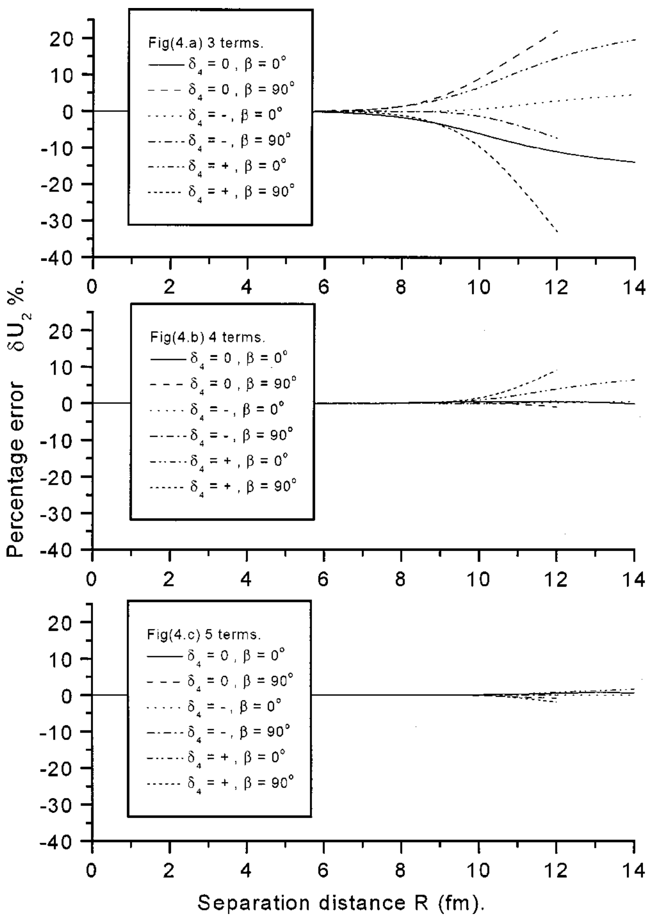

FIG. 4. Percentage of errors in the folded potential δU_2^m.

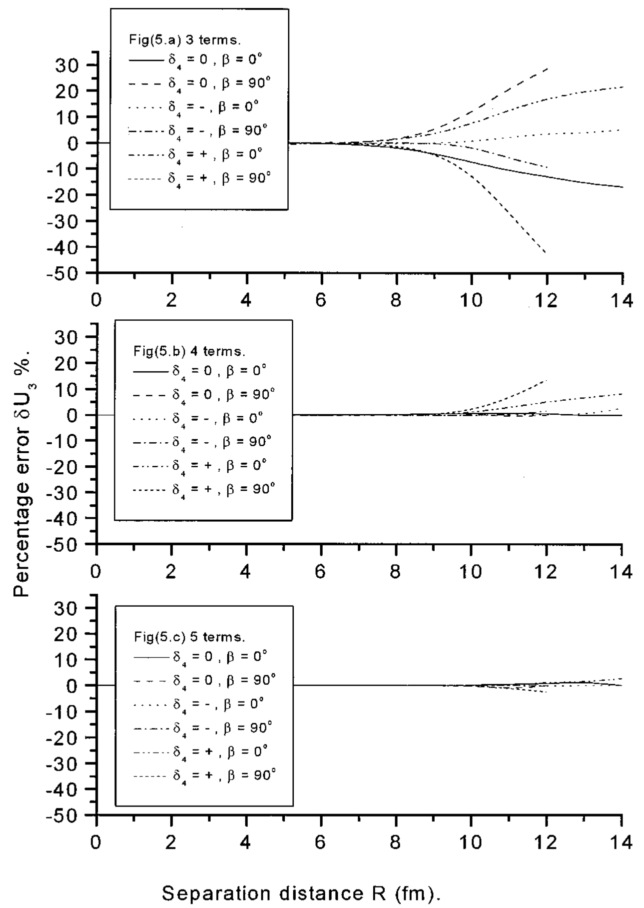

FIG. 5. Percentage of errors in the folded potential δU_3^m.

(iii) Adding the $l=6$ term of the multipole expansion, the percentage of error in all cases is reduced to less than 14%, and the limited expansion may be sufficient to represent the case of $\delta_4=0$, $\beta=0.0°$.

(iv) The multipole expansion with five terms $l\leqslant 8$ is a very good approximation for the deformed density distribution and has a few percent of error in calculating the nuclear HI potential even for the cases $\delta_4\neq 0$ and $\beta\neq 0$.

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