

Accuracy of simple folding model in the calculation of the direct part of real α – α interaction potential

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Abstract. The direct part of real α – α interaction potential is calculated in the simple folding model using density-dependent Brink–Boeker effective interaction. The simple folding potentials calculated from the short- and finite-range components of this effective interaction are compared with their corresponding double folding results obtained from the oscillator model wave function to establish the relative accuracy of the model. It is found that the direct part of real α – α interaction potential calculated in the simple folding model is reliable.

Keywords. Simple folding model; density-dependent Brink–Boeker interaction; direct part of real α – α interaction potential.

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1. Introduction

The folding model (FM) has been widely used to calculate the elastic scattering potential of heavy ions. In this model, the direct and exchange parts of the heavy-ion potential are obtained by folding the densities and density matrices of the projectile and target nuclei with the direct and exchange components of the effective nucleon–nucleon interaction, respectively. The FM calculation of the heavy-ion potential involves the evaluation of a six-dimensional integral over the intrinsic coordinates \vec{r}_1 and \vec{r}_2 of the target and projectile nucleons. The integral is conveniently evaluated by a momentum–space technique when one uses a density-independent effective interaction [1–3]. For the density-dependent effective interaction and in particular, when the density-dependent term is a fractional power of density, the evaluation of FM integral by momentum–space technique becomes much more difficult. The other convenient approach is to extend the density matrix expansion (DME) of Negele and Vautherin [4] proposed for nuclear ground state to the collision state of two nuclei involving overlap of densities of both the nuclei and employ it to

evaluate the FM integrals for direct and exchange parts of the heavy-ion potential. The evaluation becomes simple once the three-dimensional folding integral over the relative coordinate space is evaluated analytically. This extended DME method/simple folding model developed by Panda and Patra [5,6] has been used to calculate the heavy-ion optical potential from the density-dependent short-range Skyrme interaction [7] and finite-range density-dependent Brink–Boeker interaction [8].

However, the DME method [4] reproduces exact Hartree–Fock results when a short-range Skyrme interaction is used in it [9]. But, for a finite-range Brink–Boeker interaction, the DME method over binds spherical nuclei by 1 MeV per particle compared to exact Hartree–Fock calculations. Such discrepancies are almost resolved when the direct terms are calculated exactly and the DME method is applied only to the exchange terms [10]. This work in [10] suggests that the DME should only be used in the calculation of exchange contribution.

The calculation of heavy-ion potential in the energy density model (EDM), supports the validity of DME limited to the exchange part of the potential. The direct part of the heavy-ion potential calculated in EDM using the DME method is found to be unreliable [11]. Attempts have also been made in the simple folding model/extended DME method to reproduce the exchange part of the double folded heavy-ion potential [12–14] using various approximations for local Fermi momentum [15] and modified M3Y interaction [16]. The accuracy of calculating the direct part of heavy-ion potential in the simple folding model, however, remains yet to be tested.

The accuracy of the simple folding model/extended DME depends upon two factors. One is the range of the effective interaction and the other is the range of the density profile to be used in this calculation. The error to be incurred in the calculation will be more, when the range of the effective interaction is larger or when the range of the density profile is smaller. For a particular finite-range effective interaction with fixed range, the simple folding model calculation may incur maximum error in case of colliding nuclei having smallest range of density profile.

Alpha is having the smallest range of density profile among the most stable nuclei. Moreover, the calculation of α – α interaction potential has gained a renewed interest in recent years [17–22] for its importance in understanding the structure [23–25] and scattering [26–28] of α -clustered nuclei. The calculated potential can be tested in the computation of α – α scattering phase-shifts. The analysis of the phase-shift data ensures that below the reaction threshold at $E_{cm} = 17.36$ MeV, these data can be determined solely from the real part of their interaction potential. Neither the polarization potential [19] nor the imaginary potential [29] has any contribution to determine these data [30].

The density-dependent Brink–Boeker interaction have a short-range term and a finite-range Gaussian term having a range of 1.41 fm equivalent to the range of one pion exchange potential. On the other hand, the direct part of the modified M3Y interaction [16] contains two finite-range components of ranges 0.25 and 0.4 fm which are much lesser than the range 1.41 fm of density-dependent Brink–Boeker effective interaction. For a fixed range of density profile of two colliding α -particles, the error in simple folding model calculation of the direct part of real α – α potential is expected to be more, when one uses density-dependent Brink–Boeker interaction. The use of the modified M3Y interaction in this model is expected to yield less error. Thus, it is interesting to

investigate the accuracy of simple folding model in the calculation of the direct part of real α - α interaction potential using density-dependent Brink–Boeker effective interaction.

The aim of this paper, therefore, is two-fold: First, to calculate the direct part of the real α - α potential in simple and double folding models using finite-range density-dependent Brink–Boeker effective interaction and second, to study the relative accuracy of the simple folding model results.

In the following section, we outline the simple and double folding model calculations of the direct part of real α - α interaction potential from density-dependent Brink–Boeker effective interaction and present our results and discussions in §3. Finally, we report our conclusion in §4.

2. Simple folding model

2.1 Finite-range density-dependent Brink–Boeker effective interaction

The finite-range density-dependent Brink–Boeker effective interaction $v(r)$ can be given as

$$v(r) = CK_F^{1/2}\delta(r) - \frac{1}{2}V_0(1 + P)e^{-r^2/\mu^2}, \quad (1)$$

where C , V_0 and μ are the interaction parameters. P is the Majorana exchange operator. The interaction has both short- and finite-range components and acts in even states only. The finite-range is characterized by a Gaussian term with a range of 1.41 fm, identical with that of one-pion exchange two-body potential. This two-body effective interaction reproduces the structural properties of nuclear matter and finite nuclei properly, and has been used to calculate the heavy-ion interaction potential in EDM and the corresponding elastic scattering cross-sections [6].

2.2 The density matrix expansion (DME) of Negele and Vautherin

Negele and Vautherin [4] have developed an expansion for nuclear wave function density matrix in relative and centre of mass coordinates to obtain an extremely simple form for nuclear ground state energy density.

In non-relativistic dynamics, the direct V_d part of the nuclear interaction energy in the ground state of a nucleus is given as

$$\begin{aligned} V_d &= \frac{1}{2} \sum_{i < j} \langle ij | v_d | ij \rangle \\ &= \frac{1}{2} \sum_{i < j} \int \int \phi_i^*(\vec{r}_1) \phi_j^*(\vec{r}_2) v_d(|\vec{r}_1 - \vec{r}_2|) \phi_i(\vec{r}_1) \phi_j(\vec{r}_2) d^3 r_1 d^3 r_2, \end{aligned} \quad (2)$$

$$= \frac{1}{2} \int \int \rho(\vec{r}_1) \rho(\vec{r}_2) v_d(|\vec{r}_1 - \vec{r}_2|) d^3 r_1 d^3 r_2, \quad (3)$$

where \vec{r}_1 and \vec{r}_2 are the intrinsic coordinates of a pair of nucleons i and j interacting through the direct part v_d of the effective interaction v inside the nucleus. ϕ is the single-particle wave function and density $\rho(\vec{r}_1) = \sum_i \phi_i^*(\vec{r}_1) \phi_i(\vec{r}_1)$.

Using the DME proposed by Negele and Vautherin (NV), direct V_d (eq. (3)) part of the nuclear ground state energy can be obtained as

$$V_d = \frac{1}{2} \int \int \left[\rho^2(R) + \frac{1}{2} g_{sl}(k_F r) r^2 [\rho(R) \nabla^2 \rho(R) - (\nabla \rho(R))^2] \right] v_d d^3 r d^3 R. \quad (4)$$

The product of the densities $\rho(\vec{r}_1)\rho(\vec{r}_2)$ in eq. (3) is expanded in relative \vec{r} and centre of mass \vec{R} coordinates and truncated beyond the second-order derivatives to yield such simple form of the ground state energy V_d . In eq. (4), $g_{sl}(k_F r) = \frac{35}{2(k_F r)^3} j_3(k_F r)$. j_3 is the spherical Bessel function of third order and the local Fermi momentum $k_F = (1.5\pi^2\rho)^{1/3}$.

2.3 Derivation of direct part of real α - α interaction potential in the simple folding model

In the folding model, direct part V_D of the real α - α interaction potential can be expressed as

$$\begin{aligned} V_D(D) &= \sum_{\substack{i \in 1 \\ j \in 2}} \langle ij | v_d | ij \rangle \\ &= \sum_{\substack{i \in 1 \\ j \in 2}} \iint \phi_i^*(\vec{r}_1) \phi_j^*(\vec{r}_2 - \vec{D}) v_d(|\vec{r}_1 - \vec{r}_2|) \phi_i(\vec{r}_1) \phi_j(\vec{r}_2 - \vec{D}) d^3 r_1 d^3 r_2 \quad (5) \\ &= \iint \rho_1(\vec{r}_1) \rho_2(\vec{r}_2 - \vec{D}) v_d(|\vec{r}_1 - \vec{r}_2|) d^3 r_1 d^3 r_2, \quad (6) \end{aligned}$$

where D is the separating distance between the centres of the two colliding α -particles 1 and 2 shown in figure 1. It may be mentioned that similar coordinate representations have been made in obtaining eq. (6) as that of eq. (3). The interacting nucleon i is present in nucleus 1 at \vec{r}_1 and j is present in nucleus 2 at $\vec{r}_2 - \vec{D}$. ϕ and ρ are the ground-state wave function and density of the α -particle.

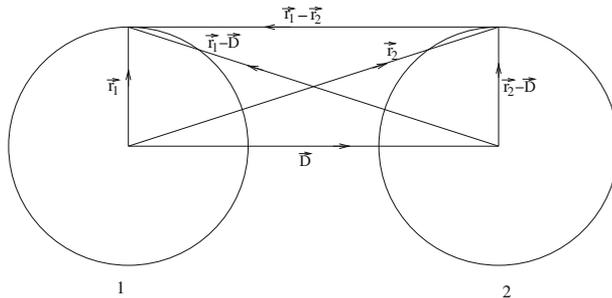


Figure 1. Coordinates used in the folding model calculation.

Calculation of real α - α interaction potential

In the simple folding model, the density matrix expansion proposed to obtain the ground state energy of a single nucleus (eq. (4)) is extended and employed to evaluate the product of densities $\rho_1(\vec{r}_1)\rho_2(\vec{r}_2 - D)$ of two colliding α -particles appearing in the folding model integral (eq. (6)) as

$$V_{SD}(D) = \iint \left[\rho_1(\vec{R})\rho_2(\vec{R} - \vec{D}) + g_{sl}(k_F r) r^2 \left[\frac{1}{4}\rho_2(\vec{R} - \vec{D})\nabla^2\rho_1(\vec{R}) + \frac{1}{4}\rho_1(\vec{R})\nabla^2\rho_2(\vec{R} - \vec{D}) - \frac{1}{2}\nabla\rho_1(\vec{R}) \cdot \nabla\rho_2(\vec{R} - \vec{D}) \right] \right] v_d(r) d^3r d^3R. \quad (7)$$

The \vec{r} -space integral in eq. (7) is obtained analytically and the six-dimensional folding model integral in eq. (7) reduces to three-dimensional integral and the computation of the direct part of real α - α interaction potential V_{SD} becomes more simple and economical,

$$V_{SD}(D) = \frac{2\pi}{D} \int R \int_{|\vec{R}-\vec{D}|}^{|\vec{R}+D|} \left\{ [428.09K_F^{1/2} - 833]\rho_1(\vec{R})\rho_2(\vec{R} - D) - X(K_F)[\rho_2(\vec{R} - D)\nabla^2\rho_1(\vec{R}) + \rho_1(\vec{R})\nabla^2\rho_2(\vec{R} - D) - 2\nabla\rho_1(\vec{R}) \cdot \nabla\rho_2(\vec{R} - D)] \right\} t dt dR. \quad (8)$$

In eq. (8), the density functional

$$X(K_F) = \int \frac{3}{8} V_0 g_{sl}(k_F r) e^{-r^2/\mu^2} r^2 d^3r. \quad (9)$$

The analytical expression of density functional $X(K_F)$ is obtained [6] as

$$X(K_F) = 115.27399 \left[1 + \sum_{i=1}^6 a_i (-k_F^2)^i \right]. \quad (10)$$

The numerical values of a_i ($i = 1-6$) are presented in table 1. This analytical expression of $X(K_F)$ reproduces their exact values over a wide range of density. In eq. (8), the first term is the direct part V_{SDS} of the potential arising out of the short-range component of the density-dependent Brink-Boeker interaction (eq. (1)) whereas, the second term plus third term is the contribution V_{SDL} arising out of the finite-range component of the same interaction (eq. (1)).

Table 1. Numerical values of a_i .

$i=$	1	2	3	4	5	6
a_i	7.688×10^{-2}	3.385×10^{-3}	1.081×10^{-4}	2.742×10^{-6}	5.804×10^{-8}	1.056×10^{-9}

2.4 Derivation of the direct part of real α - α interaction potential in the double folding model

The oscillator model wave function ϕ_{nl} in eq. (2) and the density ρ in eq. (3) of α -particle are given as

$$\phi_{nl} = C_{nl} e^{-\alpha^2 r^2 / 2} r^l F\left(1 - n, l + \frac{3}{2}; \alpha^2 r^2\right), \quad (11)$$

$$C_{nl} = \frac{1}{\Gamma\left(l + \frac{3}{2}\right)} \sqrt{\frac{2\Gamma\left(l + n + \frac{1}{2}\right)}{\Gamma(n)}} \alpha^{l + \frac{3}{2}}, \quad (12)$$

$$F(x, y, z) = 1 + \frac{x}{z} \frac{y}{1!} + \frac{x(x+1)y^2}{z(z+1)2!} + \dots, \quad (13)$$

$$\begin{aligned} \rho &= \sum |\phi_{nl}(r) Y_{lsjm}|^2 \\ &= \rho_0 e^{-\alpha^2 r^2}, \end{aligned} \quad (14)$$

where $\rho_0 = 4\alpha^3 / \pi^{3/2}$ and the oscillator width $b = 1/\alpha = 1.1931849$ fm that reproduces the best value of the RMS charge radius of 1.67 fm of α -particle [30].

The direct part of the double folding real α - α interaction potential in eq. (5) can be expressed in terms of the wave function as

$$\begin{aligned} V_{\text{FD}} &= \sum_{\substack{i \in 1 \\ j \in 2}} \iint \phi_i^* \left(\vec{R} + \frac{\vec{r}}{2} \right) \phi_j^* \left(\vec{R} - \frac{\vec{r}}{2} - \vec{D} \right) v_d(\vec{r}) \phi_i \left(\vec{R} + \frac{\vec{r}}{2} \right) \\ &\quad \times \phi_j \left(\vec{R} - \frac{\vec{r}}{2} - \vec{D} \right) d^3 r d^3 R. \end{aligned} \quad (15)$$

The six-dimensional integral over the intrinsic coordinates \vec{r}_1 and \vec{r}_2 of the pair of colliding nucleons i and j in eq. (5) has been transformed to their relative \vec{r} and centre of mass coordinate \vec{R} . Now, using the oscillator model wave function ϕ of α -particle and the density-dependent Brink–Boeker interaction, in eq. (15), we obtain the potential V_{FD} as

$$\begin{aligned} V_{\text{FD}} &= \frac{2\pi}{D} \int R \int_{|\vec{R}-\vec{D}|}^{R+D} \left[428.0999 K_F^{1/2} - \frac{2282.35}{D} \right. \\ &\quad \left. \times \int_0^\infty e^{-r^2/\mu^2} r \int_{|\vec{r}-\vec{D}|}^{r+D} e^{-\alpha^2 t_1^2/2} e^{-\alpha^2 D^2/2} t_1 dt_1 dr \right] \\ &\quad \times \rho_1(R) \rho_2(\vec{R} - \vec{D}) t dt dR. \end{aligned} \quad (16)$$

The first and second terms in eq. (15) are contributions V_{FDS} and V_{FDL} of the short- and finite-range components of the density-dependent Brink–Boeker interaction (eq. (1)), respectively towards the direct part V_{FD} of the exact double folding real α - α interaction potential.

3. Results and discussions

We have calculated the direct part of the simple folding and double folding real α - α interaction potentials V_{SDS} and V_{FDS} arising out of the short-range component of interaction v (eq. (1)) and potentials V_{SDL} and V_{FDL} from the finite-range component of the same

Table 2. Numerical values of the double folding potentials V_{FDS} and V_{FDL} and simple folding potentials V_{SDS} and V_{SDL} at different values of the separation distance D .

Potentials (MeV)	$D = 0.1$ fm	1 fm	2 fm	3 fm	4 fm
V_{FDS}	307.1	210.7	67.3	10.0	0.7
V_{SDS}	307.1	210.7	67.3	10.0	0.7
$-V_{\text{FDL}}$	380.5	284.4	117.7	27.0	3.4
$-V_{\text{SDL}}$	374.1	283.1	120.2	27.5	3.3

interaction v . In such calculations, we have used the oscillator width $b = 1.1932$ fm and related the local Fermi momentum K_{F} with the geometrical mean of the projectile and target densities, i.e., $\rho = \sqrt{(\rho_1\rho_2)}$. This approximation never exceeds the nuclear density of finite nucleus [31]. The numerical values of these calculated potentials are presented up to the separation distance $D = 4$ fm in table 2. Beyond $D = 4$ fm, all these potentials rapidly reduce to zero.

It is found that the simple folding potential V_{SDS} and the double folding potential V_{FDS} arising from the zero-range component of the density-dependent Brink–Boeker interaction (eq. (1)) are identical. In the entire range of interaction the percentage of difference between these potentials is zero. The simple folding model reproduces the direct part of the double folding α - α real potential with 100% accuracy, when a short-range two-body effective interaction is used in it.

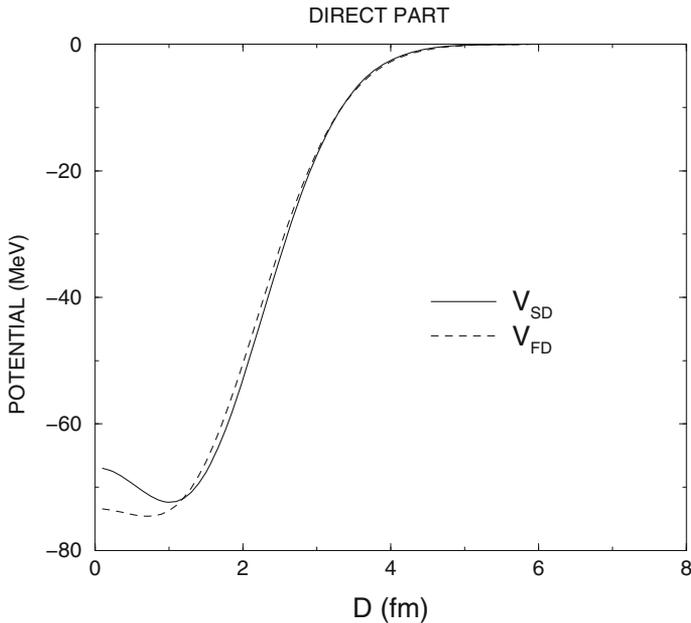


Figure 2. Comparison of the direct part of real α - α interaction potential. V_{SD} obtained in the simple folding model with their corresponding double folding potential V_{FD} .

But the difference between the simple folding potential V_{SDL} and the exact double folding potential V_{FDL} arising out of the finite-range component of the density-dependent Brink–Boeker interaction (eq. (1)) having a 1.41 fm range is found to be different at different values of the separation distance D . At $D = 0.1, 2, 3$ and 4 fm, the percentage of difference between the simple folding potential V_{FDL} and the exact double folding potential V_{SDL} are 1.68, 0.46, 2.12, 1.06 and 2.8%, respectively. The difference between these two potentials is very small. In the entire range of interaction, the simple folding model reproduces the direct part of the double folding real α – α potential within 97.1 to 99.5% accuracy when a finite-range Gaussian term having 1.41 fm range is used in it.

We have also made a comparison of direct part of the simple folding real α – α potential $V_{\text{SD}} = V_{\text{SDS}} + V_{\text{SDL}}$ (eq. (8)) with its corresponding double folding potential $V_{\text{FD}} = V_{\text{FDS}} + V_{\text{FDL}}$ (eq. (16)) in figure 2. It is found that the simple folding potential V_{SD} is very close to the double folding potential V_{FD} in the entire range of interaction.

4. Conclusion

The accuracy of the simple folding model calculation of the real part of the ion–ion interaction potential solely depends upon two factors: First, the validity of DME method to reproduce the ground state properties of the colliding nuclei and second, the approximation to be made for the local density of the composite system of the colliding nuclei that appears in simple folding model.

The DME being truncated beyond r^2 term has its own limitations that depend upon the range of two-body effective interaction and density profiles. The DME method exactly reproduces the Hartree–Fock results when a zero-range effective interaction is used in it. But, it may incur error for larger range of effective interaction and smaller range of the density profile.

The density-dependent Brink–Boeker effective interaction has a zero-range term and a finite-range term having a range of 1.41 fm identical with the range of one-pion exchange two-body potential. The α -particle has the smallest range of density profile among the stable spherical nuclei. The DME method may exhibit maximum error in the calculation of ground state properties with these inputs. Similar error can also be expected in the simple folding model calculation of ion–ion potential with such inputs. Therefore, the density-dependent Brink–Boeker interaction and α -particle are chosen to be the most suitable inputs in simple folding model to test the relative accuracy of this model in the calculation of ion–ion interaction potential.

We have calculated the direct part of real α – α potential using the density-dependent Brink–Boeker interaction, oscillator model wave function and density of α -particle in the simple and double folding models. In this calculation, we have approximated the local density of the composite system with the geometrical mean of the projectile and target densities.

It is found that simple folding model reproduces exactly the double folding results of the direct part of real α – α potential obtained from short-range component of the density-dependent Brink–Boeker interaction. The percentage of difference between the simple folding model and double folding results of the direct part of real α – α

potential obtained from the finite range (=1.41 fm) component of the density-dependent Brink–Boeker interaction is maximum up to 2.8% at the separation distance $D = 4$ fm.

Thus, the direct part of real α - α potential obtained in the simple folding model is reliable.

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