BiFold: A Python code for the calculation of double folded (bifold) potentials with density-in/dependent nucleon-nucleon interactions

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Abstract

BiFold calculates the density-dependent (DDM3Yn, BDM3Yn, CDM3Yn) or independent double folded potentials between two colliding spherical nuclei. It is written in a Python package form to give the ability to use the potentials directly in a nuclear reaction/structure code. In addition to using Woods-Saxon/Fermi or Gaussian functions, the code also allows for the definition of nuclear matter densities using pre-calculated densities in a data file. The manuscript provides an overview of the double folding model and the use of the code.

Keywords: Nuclear interaction; Double folded potentials; Density-dependent NN interactions; M3Y-interaction.

PROGRAM SUMMARY

Program Title: BiFold

CPC Library link to program files: (to be added by Technical Editor)
Developer’s repository link: https://github.com/mkarakoc/BiFold
Code Ocean capsule: (to be added by Technical Editor)
Licensing provisions: GPLv3
Programming language: Python 3.x

Nature of problem: BiFold calculates the real part of the nuclear potential between two colliding spherical nuclei by integrating a density-independent/dependent nucleon-nucleon (NN) interaction [1, 2, 3] over the nuclear matter densities of the two nuclei. The code based on M3Y Reid/Paris NN interactions [1, 2, 3] by default, but it is possible to define custom NN interactions when necessary.

Solution method: The code uses the Fourier transform method in spherical coordinates to calculate the potential. The method simplifies the sixfold integration [1] and makes the calculation a lot faster. The integration is done by default using Simpson’s integration method, but Filon’s integration method is also available.

References

[1] G.R. Satchler and W.G. Love, Phys. Rep. 55 (1979) 183.

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1. Introduction

The folded potential model [1] is a well-known model for describing the mean-field nuclear interaction between two colliding nuclei. It has been widely used in the literature [1, 2, 3, 4] since accepted as a more realistic approach than a phenomenological potential such as the well-known Woods-Saxon. The latter usually needs three free parameters to fit data, and this may create possible known ambiguities [5]. On the contrary, a folded potential usually has only one free parameter called the re-normalization factor to compensate for higher-order effects in a nuclear reaction. Folded potentials have two categories single folded (SF) potentials and double folded (DF) potentials.

The SF potential describes the interaction between two nuclei using one of the two nuclei’s densities and a phenomenological nucleon-nucleus interaction potential. The shortcomings of this treatment are density dependence, surface features, or couplings of a nuclear system are not well defined, as pointed out in the report [1] of Satchler and Love. These shortcomings make the depth of the SF potentials unrealistically deep [6, 2] to explain the rainbow scattering.

The usual DF potential between two spherical nuclei is constructed by integrating over an effective nucleon-nucleon (NN) interaction with nuclear matter densities representing nucleons of both nuclei. Although, DF potentials would overcome the shortcomings of SF potentials. Some cases for DF potentials can still overestimate the depth of the nuclear potential. Additionally, it is necessity to add the antisymmetrization-exchange effects and the density-dependent saturation effects in the effective NN interaction [2] for a more realistic nuclear potential.

The main reason for density dependence (DD) at NN interaction is the Pauli principle effects in the nuclear medium of both colliding nuclei. The DD of NN interaction has several treatments in the literature, but the code BiFold is built on the treatments of Satchler and Love [1], Kobos et al. [2], and Khoa et al. [3]. All these three treatments have the frozen density approximation while the case of Kobos et al. [2] has energy dependence, but the other two have no energy dependence.

Many studies (see the references in the present work) have used these DD treatments of NN interactions, but there are very few published codes [7, 8] to be able to reproduce the results of these works. In addition, the codes have limitations, and not all are updated regularly. For example, DFPOT [7] cannot calculate the potentials with the DDM3Y, BDM3Yn (n = 1, 2, 3), and CDM3Yn (n = 1...6) type density-dependent interactions [3]. While DFMSPTH [8] can calculate many of those, it does not support BDM3Y2, BDM3Y3 [9], and the first version of DDM3Y [2]. And it is a well-known fact results of a study must be reproducible in science. Therefore, the code BiFold will help the community in these manners.

2. The model

2.1. The usual double folded potential

It can be claimed that Coulomb potential between two spherical charges is the inspiration for the double folded potentials. And it is formulated as [1, 4]

\[ U_{DF}(\vec{R}) = \int d\vec{r}_p d\vec{r}_t \rho_p(\vec{r}_p)\rho_t(\vec{r}_t)\psi(\vec{x}), \]
Figure 1: It is the schematic representation of DF potential in Eq. (1) where $\vec{R}$ is the vector between the centers of the projectile ($p$) and the target ($t$) nuclei. $\vec{r}_p$ and $\vec{r}_t$ are the locations of the interacting parts of the nucleon distributions of both nuclei. And $\vec{s} = \vec{R} + \vec{r}_t - \vec{r}_p$ is the separation between them.

where $\rho_p$ and $\rho_t$ are charge densities, and $v(\vec{s}) = 1/\vec{s}$ interaction between charges in Coulomb potential case, while $\rho_p$ and $\rho_t$ are nuclear matter densities, and $v(\vec{s})$ is the effective NN interaction between point-like nucleons in nuclear potential case. Its schematic representation and definitions of the vectors are given in Fig. 1.

The effective NN interaction $v(\vec{s})$ is density-independent in this usual definition of the DF potentials. The medium effects are included in the calculations by changing $v(p, \vec{s}) = F(\rho) v(\vec{s})$, where $F(\rho)$ describes the density dependence of the NN interaction.

2.2. Effective density-independent NN interactions

Although BiFold can use a wide range of density-independent NN interactions in the DF potential calculations, M3Y type interactions [10, 9, 11] are defined by default in the code since they are perhaps the most widely used ones.

These interactions are called M3Y-Reid [12] and M3Y-Paris [13] effective interactions. The former is derived from the solution of the Bethe-Goldstone equation with Reid [12] soft-core interaction on a harmonic oscillator basis to obtain G-matrix. The latter is derived from a more fundamental Paris NN potential [13] to generate all components of the effective interaction [14].

Both versions of the NN interactions have direct ($v_d$) and exchange ($v_{ex}$) parts,

For M3Y-Reid:

\begin{align*}
M3Y-Reid: \\
v_d(\vec{s}) & = \left[ 7999 \frac{e^{-4s}}{4s} - 2134 \frac{e^{-2.5s}}{2.5s} \right] \text{MeV}, \\
ZR: \quad v_{ex}(\vec{s}) & = J_{ex}(E) \delta(\vec{s}) \quad \text{where} \quad J_{ex}(E) \approx -276 \left(1 - 0.005s\right) \text{MeVfm}^3, \\
FR: \quad v_{ex}(\vec{s}) & = \left[ 4631 \frac{e^{-4s}}{4s} - 1787 \frac{e^{-2.5s}}{2.5s} - 7.847 \frac{e^{-0.7072s}}{0.7072s} \right] \text{MeV}, 
\end{align*}

For M3Y-Paris:

\begin{align*}
M3Y-Paris: \\
v_d(\vec{s}) & = \left[ 11062 \frac{e^{-4s}}{4s} - 2538 \frac{e^{-2.5s}}{2.5s} \right] \text{MeV}, \\
ZR: \quad v_{ex}(\vec{s}) & = J_{ex}(E) \delta(\vec{s}) \quad \text{where} \quad J_{ex}(E) \approx -590 \left(1 - 0.002s\right) \text{MeVfm}^3, \\
FR: \quad v_{ex}(\vec{s}) & = \left[ -1524 \frac{e^{-4s}}{4s} - 518.8 \frac{e^{-2.5s}}{2.5s} - 7.847 \frac{e^{-0.7072s}}{0.7072s} \right] \text{MeV},
\end{align*}
while the direct one defines the usual nuclear interaction between nucleons. The exchange part describes the interchange (knock-on exchange) of the nucleons of the colliding nuclei [9, 11]. The DF potential will have two parts since the effective NN interactions have two parts; then Eq. (1) will have a new form

\[
U_{DF}(\vec{R}) = U_D(\vec{R}) + U_{EX}(\vec{R}) = \int \int d\vec{r}_p d\vec{r}_t \rho_p(\vec{r}_p) \rho_t(\vec{r}_t) v_d(\vec{r}_p, \vec{r}_t) + \int \int d\vec{r}_p d\vec{r}_t \rho_p(\vec{r}_p) \rho_t(\vec{r}_t) v_{ex}(\vec{r}_p, \vec{r}_t),
\]  

(8)

where \(U_D\) and \(U_{EX}\) direct and exchange folding potentials, respectively.

There are two approaches for the exchange parts of the interactions; these are zero-range (ZR) [15, 16] or finite-range (FR) [17] knock-on exchange interactions. The ZR approaches given in Eqs. (3) and (6), where \(v = E/\alpha_p\) is the projectile’s incident energy per nucleon in the laboratory frame, are widely used in the literature due to their simplicity in calculations. One needs only to put the ZR interactions in 3 or Eq. (6) to the exchange part of Eq. (8) to obtain the exchange part of the DF potential \(U_{EX}\). The depths of the ZR interactions are defined by \(J_{ex}(E)\). Determination of \(J_{ex}(E)\) is empirically done; the detailed information can be found in Refs. [15, 16, 11].

As is pointed out by Khoa [17], the exchange interaction, in general, must be nonlocal [18]. Thus, the exact numerical calculation of exchange interaction can become too complicated. A plain wave [19] approximation for the relative motion of nucleons can overcome this complication and lead to an equivalent local potential. The plain wave given in Ref. [3] is

\[
\chi(\vec{R} + \vec{s}) \approx \exp \left( \frac{i \vec{K}(\vec{R}) \cdot \vec{s}}{M} \right) \chi(\vec{R}),
\]  

(9)

where \(M = \alpha_p \alpha_t / (\alpha_p + \alpha_t)\) is the recoil factor (or reduced mass), while \(\alpha_p\) and \(\alpha_t\) are the mass numbers of the projectile and target nuclei, respectively. And \(\vec{K}(\vec{R})\) is the local momentum of the relative motion given by [18]

\[
K^2(\vec{R}) = \frac{2mM}{\hbar^2} \left[ E_{c.m.} - U_D(\vec{R}) - U_{EX}(\vec{R}) - U_C(\vec{R}) \right],
\]  

(10)

where \(E_{c.m.}\) is relative energy in the center-of-mass system, \(m\) is the nucleon mass, and \(U_C\) is the Coulomb potential. Then, local exchange potential will take the form of [17, 18, 20, 21, 22, 23]:

\[
U_{EX}(\vec{R}) = \int \int d\vec{r}_p d\vec{r}_t \rho_p(\vec{r}_p, \vec{r}_t + \vec{s}) \rho_t(\vec{r}_t, \vec{r}_t - \vec{s}) v_{ex}(\vec{s}) \exp \left( \frac{i \vec{K}(\vec{R}) \cdot \vec{s}}{M} \right),
\]  

(11)

where \(\rho_p(\vec{r}_p, \vec{r}_t + \vec{s})\) and \(\rho_t(\vec{r}_t, \vec{r}_t - \vec{s})\) are one-body density matrices [22, 23, 24] of the projectile and target nucleons. This local potential becomes an FR exchange potential when \(v_{ex}(\vec{s})\) is chosen as one of the FR interactions in Eqs. (4) or (7) (M3Y-Reid/Paris-FR). One should realize that the exchange part of Eq. (8) needs to be replaced by Eq. (11) for the FR exchange potential.

The next step in the exchange potential (Eq. (8)) is the calculation of density matrices. Although the matrices can be obtained from single-particle wave functions [18], Khoa [17] has chosen a realistic local approximation from Ref. [25]:

\[
\rho_{p,t}(\vec{r}, \vec{r} \pm \vec{s}) \approx \rho_{p,t} \left( \vec{r} \pm \frac{\vec{s}}{2} \right) \frac{1}{\left( k_{F_{p,t}}(\vec{r} \pm \frac{\vec{s}}{2}) \right)^2},
\]  

(12)
where $f_1(x) = 3(\sin x - x \cos x)/x^3$. $k_F$ is the average local Fermi momentum from Refs. [25, 26, 27, 28]:

$$k_F(\vec{r}) = \left\{ \left[ \frac{3}{2} \pi^2 \rho(\vec{r}) \right]^{2/3} + C_S \left( \frac{5}{3} \frac{\nabla \rho(\vec{r})^2}{\rho(\vec{r})^2} + \frac{5}{36} \frac{\nabla^2 \rho(\vec{r})}{\rho(\vec{r})} \right) \right\}^{1/2},$$  \hspace{1cm} (13)

where \(\rho\) is the nuclear matter densities of the projectile or the target and \(C_S\) is the strength of the Weizsäcker term, representing the surface contribution to the kinetic energy density[27]. The strength term is usually \(C_S \approx \frac{1}{36}\) in the literature, but Khoa et al. [27] have taken it as \(C_S \approx \frac{1}{36}\) for the given reasons in their work. The default value is \(C_S \approx \frac{1}{36}\) in BiFold, but the user has the option to change the value.

After this point, the FR exchange potential will have the following form [17]:

$$U_{EX}(\vec{R}) = 4\pi \int_0^\infty v_{EX}(s) s^2 ds \int f_{p,1}(\vec{r}, \vec{z}, \vec{f}_1(\vec{r} - \vec{R}, \vec{z})) j_0(K(\vec{R})) s/M d\vec{r}$$

(14)

where \(f_{p,1}(\vec{r}, \vec{z}) = \rho_{p,1}(\vec{r}) \hat{f}_1(k_{F_p,1}(\vec{r}) s)\) and \(j_0(x) = \sin x/x\). Now, the exchange potential with Fourier transforms in spherical coordinates will take the form [1, 17]:

$$U_{EX}(R) = 4\pi \int_0^\infty G(R, s) j_0(K(R) s/M) v_{EX}(s) s^2 ds,$$

(15)

where

$$G(R, s) = \frac{1}{2\pi^2} \int_0^\infty f_p(q, s) f_t(q, s) j_0(qR) q^2 dq,$$

(16)

$$f_{p,t}(q, s) = 4\pi \int_0^\infty f_{p,t}(r, s) j_0(qr) r^2 dr.$$  \hspace{1cm} (17)

Finally, it is necessary to solve a self-consistency problem to obtain the exchange part (Eq. (11)) of the double folded potential (Eq. (8)) at each radial point. Since the exchange potential (Eq. (11)) contains the local momentum of the relative motion (Eq. (10)) and \(K(\vec{R})\) depends on the total double folded potential, this problem can be solved exactly by an iterative method given in Refs. [27, 29, 22, 23].

2.3. Effective density-dependent NN interactions

The effective density-dependent NN interaction is proposed [2, 27, 28, 30] in the following form for both direct (\(v_d\)) and exchange (\(v_{ex}\)) parts:

$$v_{d,ex}(\rho, E, \vec{s}) = g(E) F_{d,ex}(\rho)v_{d,ex}(\vec{s})$$

(18)

where \(\rho\) is the overlapping density of the nuclear medium of both nuclei. \(g(E)\) is the weak intrinsic energy dependence proposed by Khoa et al. [31]. The density-dependent folding potential with an FR exchange part can be calculated by replacing this new form with \(v_d(\vec{s})\) in Eq. (8) and with \(v_{ex}(\vec{s})\) in Eq. (11). In the case of a ZR exchange part [32], it can be calculated by using the new form for both \(v_d(\vec{s})\) and \(v_{ex}(\vec{s})\) in Eq. (8).

The overlapping density for the direct part and the ZR exchange part of the folded potential has been approximated in most of the folding potential calculations [2, 33, 34, 27, 9, 35, 29, 32] as

$$\rho = \rho_p(\vec{r}_p) + \rho_t(\vec{r}_t),$$

(19)
Table 1: BiFold can calculate double folding potentials for the interactions marked with “✓” where ZR and FR stand for zero-range and finite-range exchange interactions, respectively. The × stands for not supported or non-existing interactions. The nuclear incompressibility values ($K$[MeV]) are only exist for finite range versions of the interactions [35, 29].

| Interaction names | ZR | FR | C | α | β [fm$^2$] | γ[fm$^{*}$] | n | K[MeV] | Refs. |
|------------------|----|----|---|---|---------|---------|---|--------|-------|
| DDM3Y Reid       | ✓  | ×  | 2.845 | 3.6391 | 2.9605 | 0.0 | 0 | 171 | [2, 34] |
| DDM3Y1 Reid      | ✓  | ✓  | 0.10678 | 0.0 | 0.0 | 5.1069 | 2 | 354 | [9, 35, 3] |
| DDM3Y1 Paris     | ✓  | ✓  | 1.0153 | 0.0 | 0.0 | 21.073 | 3 | 475 |       |
| DDM3Y2 Reid      | ✓  | ✓  | 1.2521 | 0.0 | 0.0 | 1.7452 | 1 | 270 |       |
| DDM3Y2 Paris     | ✓  | ✓  | 1.0664 | 0.0 | 0.0 | 6.0296 | 2 | 418 | [9, 35, 3] |
| DDM3Y3           | ✓  | ✓  | 1.0045 | 0.0 | 0.0 | 25.115 | 3 | 566 |       |
| CDM3Y1 Paris     | ✓  | ✓  | 0.3429 | 3.0232 | 3.5512 | 0.5 | 1 | 188 |       |
| CDM3Y2           | ✓  | ✓  | 0.3346 | 3.0357 | 3.0685 | 1.0 | 1 | 204 |       |
| CDM3Y3 Paris     | ✓  | ✓  | 0.2985 | 3.4528 | 2.6388 | 1.5 | 1 | 217 | [29, 3] |
| CDM3Y4           | ✓  | ✓  | 0.3052 | 3.2998 | 2.3180 | 2.0 | 1 | 228 |       |
| CDM3Y5           | ✓  | ✓  | 0.2728 | 3.7367 | 1.8294 | 3.0 | 1 | 241 |       |
| CDM3Y6           | ✓  | ✓  | 0.2658 | 3.8033 | 1.4099 | 4.0 | 1 | 252 |       |
| M3Y Reid         | ✓  | ✓  | usual density-independent M3Y |       |       |       |     |       | 1, 17, 32 |
| M3Y Paris        | ✓  | ✓  |       |       |       |       |     |       |       |

since it permits the separation of variables in the integrals of Eqs. (8) and (11). The overlapping density for the FR exchange part of the folded potential has been assumed [2, 33, 34, 27, 9, 35, 29, 32] as

$$\rho = \rho_p(\vec{r}_p + \frac{\varepsilon}{2}) + \rho_t(\vec{r}_t - \frac{\varepsilon}{2}).$$

(20)

The code can calculate double folding potentials for the interactions marked with a “✓” in Table 1. The density dependence of these interactions is defined by $F(\rho)$ in Eq. (18). Different versions of 18 are proposed in the Refs. [2, 31, 9, 29]. In a more recent study by Khoa et al. [3], these different versions of $F(\rho)$ merged into one formula;

$$F(\rho) = C[1 + \alpha \exp(-\beta \rho) - \gamma \rho^\kappa].$$

(21)

The parameters of this formula are given in Table 1 other than the original DDM3Y [2] since its parameters are energy-dependent. The values of these energy-dependent parameters can be obtained from the Refs. [2, 34].

The final part of the density-dependent NN interaction (Eq. (18)) is $g(E)$. It is $g(E) = 1$ for the original DDM3Y [2] since $g(E)$ does not exist for this interaction. For the remaining density-dependent interactions in Table 1, $g(E) \approx 1 - \kappa \varepsilon$, where $\kappa = 0.002$ and $\varepsilon = E/a_p$ is energy (in MeV) per nucleon.

3. The code

The code structure of BiFold code given in Fig. 2 on the left. The bold ones are directories, and the rest are Python files in the given file structure. The two sub-directories in the bifold direc-
An example Python file for calculating a density-independent double potential using M3Y-Reid NN interaction with the ZR exchange part (see Eqs. (2) and (3)) for an $\alpha^{\text{40}}\text{Ca}$ elastic scattering:

```python
from bifold import *

r = mesh(zero, 10, 0.05) # fm
q = mesh(zero, 3, 0.05) # fm^-1

e_lab = 141.7 # MeV
a_proj = 4

rho_p = f2p*gaussian(r, 0.4229, (1/0.7024)**0.5)  # fm^-1
rho_d = f2p*fermi(r, 0.169, 3.60, 0.523)

u = u_m3y_reid_zr(e_lab, a_proj, rho_p, rho_d, r, q)

title = "a + 40Ca @ Elab = 141.7 MeV using M3Y-Reid/ZR"
print_all(u, r, q, title=title)
plot_potentials(u, r, part="all")
```

Figure 2: The file tree structure of BiFold code is on the left. The bold ones are directories, and the rest are Python files. An example Python file to calculate a double folding potential for an $\alpha^{\text{40}}\text{Ca}$ elastic scattering on the right.
scattering is on the right side of Fig. 2. And the results of the calculation are shown in Figs. 3 and 4. One may agree that the code is easy to understand. The first line of the Python code imports BiFold since it is a Python package. On the third and fourth lines, the \texttt{mesh} functions define the numerical integration grids for \( r \) = zero fm to \( r \) = 10 fm with 0.05 fm steps and \( q = \text{zero} \text{ fm}^{-1} \) to \( r \) = 3 fm\(^{-1} \) with 0.05 fm\(^{-1} \) steps where \( \text{zero} = 1 \times 10^{-10} \). The sixth and seventh lines are the laboratory energy (\( e_{\text{lab}} \)) and the atomic mass number (\( a_{\text{proj}} \)) of the projectile (\( a \) = particle), respectively. The ninth and tenth lines are the nuclear matter densities of the projectile (\( R \alpha \)) and the target (\( R \alpha \)) nuclei, respectively. The twelfth line is the double folding calculation in Eq. (8) for M3Y-Reid NN interaction with the ZR exchange part (see Eqs. (2) and (3)). The rest of the file is optional if one needs to print (Fig. 3) the calculation information and draw (Fig. 4) the potentials versus radial distance between the two nuclei. This code is a simple example of how to use BiFold to calculate a double-folded potential. The related GitHub page has the BiFold code, a more detailed user guide, and more examples.

Figure 3: It is the output of the double folding potential calculation for the \( a + ^{40}\text{Ca} \) elastic scattering.
Figure 4: It is the double folding potential [dash-dot] with direct [solid] and exchange [dash] parts for the $\alpha$+$^{40}$Ca elastic scattering.

The output of the BiFold calculation shown in Fig. 3 gives individual information about the potentials and the functions used in the calculations. This individual information from left to right contains a Python dictionary key, name of the function/potential, multi-polarity (L), normalization (norm) and re-normalization (renorm), volume integrals (vol2 and vol4), and mean square radii (msr). The output also contains printout of the calculated potential $U_R$ versus radial distance $R$ between two nuclei.

The dictionary keys `func_i`, `func_r` and `func_q` store the information about the function, numeric values of the function at every point defined by mesh($r_{\text{min}}$, $r_{\text{max}}$, $dr$), and numeric values of the function’s Fourier transform at every point defined by mesh($q_{\text{min}}$, $q_{\text{max}}$, $dq$), respectively. The output does not list these keys. The keys total, direct and exchange are to reach total, direct and exchange individual parts of the calculations under the previous keys. And $u_R$, $\rho_p$, $\rho_t$, and $vnn$ keys store information about every individual part under the previous keys. Finally, one can reach the information tabulated in the output by using L, norm, renorm, vol2, vol4 and msr keys. For example, using `func_i`, `direct` and `rho_p` keys in the given order will produce the following output about the density of the projectile nucleus in the example code in Fig. 2:

```python
input: u["func_i"]['direct']['rho_p']
output: {"name": "f2prim_gaussian", 'L': 0, 'norm': None, 'renorm': 1.0, 'vol2': 4.000237160, 'vol4': 6.542647693, 'msr': 2.135535308}
```

The following formula defines the volume integrals for all radial dependent functions and potentials,

$$vol(n + 2) = \text{renorm} \, 4\pi \int f(r)r^{n+2}dr.$$  \hspace{1cm} (22)

If the value of `norm` is `None`, then $\text{renorm} = 1$, otherwise if `norm` is a real number, then $\text{renorm}$ is,

$$\text{renorm} = \text{norm} \left[ 4\pi \int f(r)r^{n+2}dr \right]^{-1}.$$  \hspace{1cm} (23)

The mean square radii (msr) of all radial dependent functions and potentials are $\langle r^2 \rangle = \text{vol4}/\text{vol2}$. 

![Graph showing the double folding potential with direct and exchange parts for $\alpha$+$^{40}$Ca elastic scattering.](image-url)
4. Test cases

This section compares BiFold computations to three examples to demonstrate the code’s reliability. The first one is an analytical calculation, and the second one is a numerical calculation using DFPOT [7]. And the work of Khoa et al. [35] is the last one. One can assume that the examples are reasonably accurate since the first example is an exact solution to the double folding integrals, the second example is a published code used and tested many times in the literature, and the final one is a reliable published work. Therefore, these examples are reference calculations to use in the following formula,

$$\xi^2 = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{U_A(R_i) - U_B(R_i)}{U_A(R_i) + U_B(R_i)} \right)^2.$$  \hspace{1cm} (24)

This formula defines a mean relative error (mre) [8] for comparing BiFold calculations with reference calculations where $U_A$ and $U_B$ are the reference and the present double folding potentials with the radial distance $R_i$, respectively. It is better if $\xi^2$ is getting closer to zero, as it will mean that the results of both computations are getting more consistent. The results of the mre calculations are in Table 4, and the details of the test cases are in the following sections.

Table 4: The mean errors, defined by Eq. (24), are given for the three test cases. The cases are compared with BiFold’s calculations using both Simpson’s and Filon’s integration.

| Integration method of BiFold | Analytical $\rho_{max} = 3$ fm$^{-1}$ | Analytical $\rho_{max} = 10$ fm$^{-1}$ | DFPOT | Khoa et al. [35] |
|-----------------------------|--------------------------------------|---------------------------------------|-------|-----------------|
| Simpson                     | total $\xi^2$                        | $1.16 \times 10^{-7}$                | $1.31 \times 10^{-7}$ | $6.5 \times 10^{-5}$ |
|                            | direct $\xi^2$                       | $1.9 \times 10^{-7}$                 | $8.13 \times 10^{-5}$ | $6.65 \times 10^{-3}$ |
|                            | exchange $\xi^2$                     | $2.12 \times 10^{-6}$                | $1.4 \times 10^{-7}$  | $2.48 \times 10^{-5}$ |
| Filon                      | total $\xi^2$                        | $1.16 \times 10^{-7}$                | $1.31 \times 10^{-7}$ | $6.5 \times 10^{-5}$ |
|                            | direct $\xi^2$                       | $1.9 \times 10^{-7}$                 | $8.13 \times 10^{-5}$ | $6.65 \times 10^{-3}$ |
|                            | exchange $\xi^2$                     | $2.12 \times 10^{-6}$                | $1.4 \times 10^{-7}$  | $2.48 \times 10^{-5}$ |

4.1. BiFold vs. analytical calculation

In this case, $\alpha + \alpha$ scattering with projectile energy 50 MeV in the laboratory system is in consideration. Satchler and Love [1] suggested a Gaussian shaped nuclear matter distribution for an $\alpha -$ particle is

$$\rho(r) = 0.4229 \, e^{-0.7024r^2} \, \text{fm}^{-3},$$  \hspace{1cm} (25)

with a mean square radius $\langle r^2 \rangle = 2.1355$ fm$^2$. A new nuclear matter distribution for the $\alpha -$ particle is

$$\rho(r) = 2.12 \, e^{-2.3705r} \, \text{fm}^{-3},$$  \hspace{1cm} (26)

proposed using the msr value since the previous one does not allow to obtain an analytical solution. Therefore, the reason for choosing this distribution is to obtain an exact analytical double-folded potential since the density-independent NN effective interaction (M3Y-Reid, Eq. (2) also has a similar mathematical form. Then this is easily achieved by using the Fourier transform.
techniques as usual [1] for the double folding integral given in Eq. (8), but this time with an analytical integration. Thus, the analytical double-folded potential with both direct and ZR exchange NN interactions included is

\[
U(R) = \frac{1}{R} 2747 \left( e^{-4R} - 31323.3246 e^{-2.5R} - 10.729866914 e^{-2.3705R} \times \right. \\
\left. [R^3 - 24.345R^2 + 377.89705R - 2919.17177] \right). 
\]  

(27)

Both computations agree very well, as supported by the \(\xi^2\) values in Table 4 and shown in Fig. 5a. The \(\xi^2\) values are almost the same for both integration methods. There is a caveat to be careful of about this case. The effective NN interaction and the new nuclear matter distribution slowly go to zero when \(r\) goes to infinity, contrary to the Gaussian-shaped density in Eq. (25). This leads to the problem shown in Fig. 5b, where \(q_{\text{max}} = 3 \text{ fm}^{-1}\) is not enough to obtain a numerically accurate solution. Therefore it was necessary to raise \(q_{\text{max}}\) to 10 \text{ fm}^{-1} in this case while this value of \(q_{\text{max}}\) is usually enough most of the time, as mentioned in Ref. [7]. This problem illustrates it is better to make a consistency check by raising the value of \(q_{\text{max}}\) till the calculation reaches a saturation point where the potential does not change anymore.

![Figure 5: The full circles, up triangles, and down triangles are the calculations of the total, direct and exchange parts of the analytically calculated double folding potentials, respectively. The solid lines are the computations using BiFold.](image)

4.2. BiFold vs. DFPOT

This test case compares the two codes for an \(\alpha + ^{40}\text{Ca}\) elastic scattering system where the energy of the \(\alpha\) projectile is 141.7 MeV in the laboratory system. The effective NN interaction is for both codes is the density-independent M3Y-Paris with the ZR exchange part given in Eqs. (5) and (6). BiFold can perform the calculation for this case by changing ‘\(\text{u.m3y.reid.zr}\)’ to ‘\(\text{u.m3y.paris.zr}\)’ in the twelfth line of Python code shown in Fig. 2.

The nuclear matter density for \(\alpha - \) particle is in Eq. (25), and the density [34] of \(^{40}\text{Ca}\) is

\[
\rho(r) = 0.169 \left[ 1 + \exp \left( \frac{r - 3.60}{0.523} \right) \right]^{-1} \text{ fm}^{-3}, 
\]  

(28)

with a msr value of \(\langle r^2 \rangle = 11.553 \text{ fm}^2\). As seen in Fig. 6, the computations of both codes are in very well agreement with each other, and the \(\xi^2\) values in Table 4 also support the claim.
Figure 6: The full circles, up triangles, and down triangles are the calculations of the total, direct and exchange parts of
the double folding potentials using DFPOT [7], respectively. The solid lines are the computations using BiFold.

4.3. BiFold vs. Khoa et al.’s calculation

The $^{16}$O+$^{16}$O elastic scattering system at several incident energies was studied by Khoa et al. [35] using various density-dependent M3Y-Paris-based NN interactions. The case chosen for the comparison is the one at 250 MeV incident energy. And the effective NN interaction used for the double folding potential is the BDM3Y1-Paris NN interaction with the FR exchange part. The calculations of Khoa et al. [35] were obtained by digitizing the related figure in the reference with the help of the programs Inkscape [41] and Engauge Digitizer [42].

The nuclear matter density of the $^{16}$O nuclei with the msr value $\langle r^2 \rangle = 6.625 \text{ fm}^2$ [34, 35] is

$$\rho(r) = 0.181 \left[1 + \exp\left(\frac{r - 2.525}{0.45}\right)\right]^{-1} \text{ fm}^{-3}. \quad (29)$$

Since BDM3Y1 is a density-dependent NN interaction, the double folding integral in Eq. (11) has to be solved to obtain the potentials in Fig. 7. This integral contains the Coulomb potential between the two nuclei through the local momentum $\vec{K}$ of the relative motion. The Coulomb potential modeled for uniformly charged spherical nuclei is

$$U_C(R) = z_p z_t e^2 4 \pi \varepsilon_0 \left(\frac{\pi}{2 R_C}\right) \left[3 - \left(\frac{g}{R_C}\right)^2\right] \left\{ \begin{array}{ll} \left(1 - \frac{R}{R_C}\right)^{-1} \quad (R > R_C) \\ \left(1 + \frac{R}{R_C}\right)^{1/3} + \left(1 + \frac{R}{R_C}\right)^{1/3} \quad (R \leq R_C) \end{array} \right. \quad (30)$$

used in the calculations where $z_p$, $z_t$ are proton numbers of the projectile and the target, respectively. The Coulomb radius is $R_c = 1.405 \left(a_p^{1/3} + a_t^{1/3}\right) \text{ fm}$.

As can be seen from the $\xi^2$ values in Table 4 and the potentials in Fig. 7, BiFold is also consistent with the final reference work. It is important to note here that the comparison is made till 5.6 fm in this case since the resolution of the digitized figure [35] was not enough to recover the data with enough precision.
Figure 7: The full circles, up triangles, and down triangles are the calculations of the total, direct and exchange parts of the double folding potentials from Khoà et al. [35], respectively. The solid lines are the computations using BiFold.

Declaration of competing interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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