Chapter 4

Universal function of nuclear proximity potential for Skyrme nucleus-nucleus interaction in semiclassical approach

4.1 Introduction

Recently [1], Gupta et al. calculated the spin-orbit density part of the Skyrme nucleus-nucleus interaction, approximated as the nuclear proximity potential, within the semiclassical Extended Thomas-Fermi (ETF) approach. This has been possible because in the semiclassical formulation of Skyrme energy density functional (SEDF) [2-5], both the kinetic energy density $\tau$ and the spin-orbit density $\mathcal{J}$ are expressed as functions of nucleon or nucleus density, $\rho_q(\vec{r})$ $q=n$ or $p$ or $\rho(\vec{r})$$(=\rho_n(\vec{r})+\rho_p(\vec{r}))$, alone. Earlier, in the microscopic shell model approach, introduced by Vautherin and Brink [6] for spherical (doubly closed shell) nuclei and extended by Gupta and collaborators [7] to un-closed shell nuclei, such a solution in terms of proximity potential could be worked out only for spin-saturated ($\mathcal{J}=0$)
nuclei or, equivalently, the spin-orbit density independent part of the interaction potential $V_p(R)$ [7, 8] since it depends on nuclear densities $\rho_i$, $i=1,2$ for two nuclei. The same for spin-orbit density dependent interaction potential $V_j(R)$ could not be done [9] because in this formalism [6, 7] $V_j(R)$ depends on the filling of shell model states. Hence, the new alternative of using the semiclassical ETF formulation of the SEDF calls for to express the total Skyrme nucleus-nucleus interaction potential $V_{N}(R)$ (sum of both the spin-orbit density independent $V_p(R)$ and the spin-orbit density dependent $V_j(R)$ parts) as a proximity potential, i.e., to obtain the universal function $\phi(D)$ of proximity potential for SEDF in ETF formalism, with $D$ as the separation distance between the two nuclear surfaces. Since $V_p(R)$ and $V_j(R)$ are known from microscopic formalism to behave differently (one attractive and another repulsive; see, e.g., Ref. [9]), for the semiclassical ETF formalism also we obtain $\phi(D)$ as a sum of their two independent universal functions $\phi_p(D)$ and $\phi_j(D)$. This is attempted for the first time here in this chapter.

The semiclassical approach at the ETF level, with $\hbar$ as its order parameter, contains contributions of orders higher than two for both the kinetic energy density $\tau(\vec{r})$ and spin-orbit density $J(\vec{r})$ [3-5], but we limit here up to second order contributions (denoted ETF2) for reasons of their being enough for numerical convergence [5]. This already means going beyond the von Weizsäcker correction for kinetic energy density (see, e.g., Ref. [8]) and one order higher for spin-orbit density. Some authors [10] have shown that the fusion barriers for heavy systems ($Z_1Z_2 > 680$) are sensitive to the next higher order term (the $\hbar^4$ term, denoted ETF4), which happens because the surface diffuseness obtained in their restricted density variational method fall short of the Skyrme-HF estimates, and hence, in their later work [11], they also use the ETF2 for heavy and superheavy systems. In the present work, we use the experimental data for surface diffuseness and, in view of the numerical convergence [5], the ETF2 is considered enough. We further show the importance of surface diffuseness parameters $a_{oi}$ (and half-density radii $R_{oi}$, $i=1,2$) in fitting the
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Figure 4.1: The spin-orbit density independent function $\phi_p(D)$ and spin-orbit density dependent function $\phi_s(D)$ calculated on semiclassical ETF approach for various pairs of colliding nuclei (scattered points), and the corresponding parameterized universal functions of proximity, Eqs. (4.1) and (4.2), shown as solid lines for (a) SII, (b) SIII, (c) SIV and (d) SkM* Skyrme forces.

fusion cross-sections.

The chapter is organized as follows. Our illustrative calculations and discussion of results are presented in Section 4.2. This section also illustrate our use of the derived proximity potential to calculate the fusion cross-sections, and its fitting in terms of the constants of universal function. Finally, a summary of our results is given in Section 4.3.
4.2 Calculations and discussion of the results

First of all, we look for the universality of the nuclear proximity functions $\phi_P(D)$ and $\phi_J(D)$ for use of various Skyrme forces SII, SIII, SIV, SkM*, SLy4, SKa, MSK1 and SGII, selected randomly (the original Skyrme force S could not be used here since the spin-orbit strength $W_0=0$ in this case). This is illustrated in Fig. 4.1 for SII, SIII, SIV, and SkM*, and in Fig. 4.2 for SLy4, SKa, MSK1 and SGII forces, where the two functions $\phi_P(D)$ and $\phi_J(D)$, calculated for some 35 cases of colliding pairs of nuclei with compound nucleus mass up to $A=294$, using both the kinetic energy density and spin-orbit density up to second order, are plotted as scattered points. We notice three interesting results: (i) for each force, the two functions

Figure 4.2: Same as for Fig. 4.1, but for (a) SLy4, (b) SKa, (c) MSK1 and (d) SGII Skyrme forces.
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Figure 4.3: The two contributing terms $V_p(R)$ and $V_j(R)$ of nucleus-nucleus interaction potential $V_n(R) (= V_p(R) + V_j(R))$ for an illustrative reaction $^{32}$S+$^{40}$Ca, using various Skyrme forces, calculated by using the “exact” integrals, Eqs. (2.90) and (2.88), and the parameterized universal functions, Eqs. (4.1) and (4.2).

show altogether different characteristics, the $\phi_p(D)$ being mainly attractive and $\phi_j(D)$ mainly repulsive; (ii) the maximum or peak value for the spin-orbit density dependent function $\phi_j(D)$ is always at the touching configuration $D=0$, while for the spin-orbit density independent function $\phi_p(D)$ the minimum is always at $D > 0$; (iii) the general behaviors of both the functions are, independently, each of the universal functions and can be parameterized for all the above mentioned Skyrme forces, like in Ref. [12], for spin density independent part, as

$$
\phi_p(D) = \begin{cases} 
-\phi^p_b \exp\left[-a(D - D_0)^{1.07}\right] & \text{for } D \geq D_0 \\
-\phi^p_b + b(D - D_0)^2 & \text{for } D \leq D_0 
\end{cases}
$$

(4.1)
Table 4.1: Constants obtained for the parameterized universal functions of spin-orbit-density independent part $\phi_P$ and spin-orbit-density dependent part $\phi_J$ [Eqs. (4.1) and (4.2)], using different Skyrme forces.

<table>
<thead>
<tr>
<th>Force</th>
<th>$\phi_P^0$</th>
<th>$D_0$</th>
<th>$a$</th>
<th>$b$</th>
<th>$\phi_J^0$</th>
<th>$c$</th>
<th>$d$</th>
<th>$e$</th>
<th>$f$</th>
<th>$g$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$SHI$</td>
<td>1.28</td>
<td>0.35</td>
<td>0.46</td>
<td>0.80</td>
<td>0.164</td>
<td>0.43</td>
<td>0.012</td>
<td>0.139</td>
<td>0.049</td>
<td>0.005</td>
</tr>
<tr>
<td>$SHII$</td>
<td>1.28</td>
<td>0.30</td>
<td>0.44</td>
<td>1.00</td>
<td>0.259</td>
<td>0.44</td>
<td>0.029</td>
<td>0.263</td>
<td>0.092</td>
<td>0.009</td>
</tr>
<tr>
<td>$SIV$</td>
<td>1.37</td>
<td>0.26</td>
<td>0.43</td>
<td>0.80</td>
<td>0.289</td>
<td>0.44</td>
<td>0.013</td>
<td>0.220</td>
<td>0.079</td>
<td>0.008</td>
</tr>
<tr>
<td>$SkM^*$</td>
<td>1.40</td>
<td>0.14</td>
<td>0.35</td>
<td>0.55</td>
<td>0.313</td>
<td>0.44</td>
<td>0.052</td>
<td>0.346</td>
<td>0.121</td>
<td>0.012</td>
</tr>
<tr>
<td>$SLy4$</td>
<td>1.40</td>
<td>0.15</td>
<td>0.41</td>
<td>0.45</td>
<td>0.249</td>
<td>0.46</td>
<td>0.018</td>
<td>0.222</td>
<td>0.077</td>
<td>0.008</td>
</tr>
<tr>
<td>$SKa$</td>
<td>1.40</td>
<td>0.18</td>
<td>0.40</td>
<td>0.60</td>
<td>0.236</td>
<td>0.44</td>
<td>0.014</td>
<td>0.196</td>
<td>0.069</td>
<td>0.007</td>
</tr>
<tr>
<td>$MSK1$</td>
<td>1.35</td>
<td>0.14</td>
<td>0.39</td>
<td>0.60</td>
<td>0.312</td>
<td>0.50</td>
<td>0.052</td>
<td>0.409</td>
<td>0.142</td>
<td>0.014</td>
</tr>
<tr>
<td>$SGII$</td>
<td>1.20</td>
<td>0.18</td>
<td>0.38</td>
<td>0.50</td>
<td>0.209</td>
<td>0.50</td>
<td>0.017</td>
<td>0.211</td>
<td>0.074</td>
<td>0.008</td>
</tr>
</tbody>
</table>

and for spin-orbit density dependent part, as

$$
\phi_J(D) = \begin{cases} 
\phi_J^0 \exp[-cD^2] & \text{for } D \geq 0 \\
\phi_J^0 - dD - eD^2 - fD^3 - gD^4 & \text{for } D \leq 0
\end{cases} \quad (4.2)
$$

with constants $\phi_P^0$, $D_0$, $b$, and $b$ of $\phi_P(D)$ and $\phi_J^0$, $c$, $d$, $e$, $f$ and $g$ of $\phi_J(D)$ for different Skyrme forces obtained as given in Table 4.1. The two parameterized universal functions of proximity, $\phi_P(D)$ and $\phi_J(D)$, are shown as solid lines in Figs. 4.1 and 4.2 for all the forces studied here. Apparently, Eqs. (4.1) and (4.2) give the average representations of $\phi_P(D)$ and $\phi_J(D)$, respectively, with $\phi_P^0$ as the maximum attraction of $\phi_P(D)$ at $D = D_0$ and $\phi_J^0$ as the maximum repulsion of $\phi_J(D)$ at $D=0$.

Note, in Eq. (4.1) the power 1.67 (=5/3) of exponential, instead of the generally used power 2, gives a better representation of calculations (scattered points) in the physically more interesting region for heavy ion collisions, the surface region of interaction potential (equivalently, the universal function here).

Figure 4.3 shows the corresponding two interaction potentials $V_P(R)$ and $V_J(R)$, the spin-orbit density independent and spin-orbit density dependent parts, for an illustrative $^{32}$S+$^{40}$Ca reaction, calculated by using the actual integrals [Eq. (2.88) and
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"Exact"  -------Empirical (\(R_0, a\))  
-------Fitted (\(R^*, a_q\))

Parameterized

Figure 4.4: The total interaction potential \(V_T(R)\) for \(^{64}\text{Ni}+^{64}\text{Ni}\) reaction for the cases of "exact" and parameterized universal functions, using the empirically determined parameters \(R_{01} = R_{02} = R_0\) and \(a_{01} = a_{02} = a_0\) (thick solid and dashed lines) and ones fitted to data on cross-sections (thin solid and dashed lines) for SIV Skyrme force.

(2.90)], marked “exact”, and the parameterized universal functions [Eqs. (4.1) and (4.2)]. We find that the parameterized universal functions reproduces the “exact” potentials with in less than \(\sim 1\) MeV of difference in the surface region, including at the maximum attraction (repulsion) for \(V_p\) (\(V_j\)). This is further illustrated in the following for fusion cross-sections.

Finally, adding the Coulomb interaction term to the nuclear interaction potential \(V_N(R)\), we get the total interaction potential given by eq. (2.98) which gives the barrier height \(V_B\) and position \(R_B\), illustrated in Fig. 4.4 for \(^{64}\text{Ni}+^{64}\text{Ni}\) reaction, using both the “exact” formalism [Eq. (2.88) and (2.90), solid thick line] and the
Figure 4.5: The fusion cross-section for the reaction $^{64}\text{Ni}+^{64}\text{Ni}$, using Skyrme force SIV, calculated for the cases of "exact" and parameterized universal functions, using the empirically determined parameters $R_{01} = R_{02} = R_0$ and $a_{01} = a_{02} = a_0$ (thick solid and dashed lines) and ones fitted to data on cross-sections (thin solid and dashed lines), compared with experimental data [13].

parameterized one [Eqs. (4.1) and (4.2), dashed thick line] for an illustrative Skyrme force SIV. Note that in "exact" calculations, the central radius $R_{01} = R_{02} = R_0$ and surface diffuseness $a_{01} = a_{02} = a_0$ for $^{64}\text{Ni}$ are taken from the empirically determined polynomials (2.94), with $T$-dependence as in Eq. (2.95), respectively. Using the above information on $V_B$, $R_B$ and the curvature $\hbar\omega_0$ of the interaction potential $V_T(R)$ from Fig. 4.4 in Wong’s formula as given by eq. (2.102) (also see Ref. [14]), we get the cross-sections as a function of the center of mass energy $E_{c.m.}$. $\hbar\omega_0$ is obtained for an inverted harmonic oscillator fit to the curvature in $V_T(R)$ at the top of the barrier.
Fig. 4.5 shows a comparison of our above mentioned calculation for fusion cross-sections with the experimental data [13] for $^{64}\text{Ni}+^{64}\text{Ni}$ reaction. The temperature $T$ (in MeV) is related to $E_{\text{c.m.}}$, via the compound nucleus excitation energy $E_{\text{CN}}^*$ and Q-value of the incoming channel, as given by eq. (2.18). We notice in Figs. 4.4 and 4.5 that the two calculations ("exact" and parameterized one, with empirical $R_{0i}$ and $a_{0i}$) give identical results, though the fit to data in Fig. 4.5 is reasonable only at top two energies. Thus, the parameterized universal functions are shown to be a useful replacement of the lengthy "exact" calculations of SEDF in semiclassical ETF method.

Table 4.2: Empirical and fitted $(R_0, a_0)$ and $(\phi_p^0, a)$ for $^{64}\text{Ni}$ used in "exact" and parameterized formalisms of SEDF in semiclassical ETF method for Skyrme force SIV.

<table>
<thead>
<tr>
<th></th>
<th>Empirical</th>
<th>Fitted</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(R_0, a_0)$</td>
<td>(4.212, 0.556)</td>
<td>(4.90, 0.440)</td>
</tr>
<tr>
<td>$(\phi_p^0, a)$</td>
<td>(0.556, 0.440)</td>
<td>(1.00, 0.69)</td>
</tr>
</tbody>
</table>

Regarding the nature of fits in Fig. 4.5 for empirical $(R_0, a_0)$, first we note that Wong Formula, with its approximate summation over angular momentum variable $\ell$, is not the best choice. We have used it here simply for a comparative study between the "exact" and parameterized formalisms. Secondly, in a recent work [15], we showed that such a failure of Wong formula is related to the choice of parameters $R_{0i}$ and $a_{0i}$ of SEDF, found related to the adjustment of the height and curvature of the barrier. In the case of the parameterized universal functions, the same job of adjusting the barrier height and its curvature parameter $\hbar\omega_0$ is shown to be done by the constants $\phi_p^0$ and $a$, the maximum attraction of spin-orbit independent universal function $\phi_p(D)$ and its surface parameter $a$. This is illustrated in Fig. 4.4 for the interaction potentials obtained for both the "exact" and parameterized formalisms.
(thin solid and dashed lines) for the best fit to the data in Fig. 4.5 (thin solid and dashed lines). The empirical versus fitted \((R_0, a_0)\) and \((\phi_P, a)\) are given in Table 4.2. We notice that the fits in Fig. 4.5 are improved considerably for a small change in constants of the model, and that the fits in two cases (exact and parameterized) are nearly of the same quality. The interesting result of lowering of the barrier and changed curvature are more than evident in Fig. 4.4, supporting the recent work of Misicu and Esbensen [16] for M3Y potential and of the dynamical cluster-decay model (DCM) and Wong model of Gupta and collaborators [17,18].

4.3 Summary

The nucleus-nucleus interaction potential, calculated in Skyrme energy density functional method by using the semiclassical Extended Thomas-Fermi approach, is expressed in terms of the universal function of proximity potential. This is obtained as a sum of the spin-orbit density independent universal function \(\phi_P(D)\) and the spin-orbit density dependent universal function \(\phi_J(D)\), respectively, since the two parts show opposite behaviors, \(\phi_P(D)\) mainly attractive and \(\phi_J(D)\) mainly repulsive. The semiclassical expansions of both the kinetic energy density and spin-orbit density are included up to second order and the two parameter Fermi density with its two parameters, the half-density radius \(R_{0i}\) and surface diffuseness \(a_{0i}\), fitted to experiments is used for the nuclear density. The analytical expressions obtained for the universal functions give the “exact” nuclear interaction potential with in less than \(\sim 1\) MeV, both at the maximum attraction and surface region of interest for heavy-ion collisions. Application of the parameterized universal function to fusion cross-sections show the possibility of modifying the barrier characteristics, required for below barrier energies, in terms of its constants \((\phi_P, a)\), similar to the constants \((R_{0i}, a_{0i})\) of Fermi density which modify the “exact” barrier determined in Skyrme energy density functional based semiclassical Extended Thomas-Fermi method.
Bibliography


