Mean-Field Description of Fusion Barriers with Skyrme’s Interaction

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Fusion barriers are determined in the framework of the Skyrme energy-density functional together with the semi-classical approach known as the Extended Thomas-Fermi method. The barriers obtained in this way with the Skyrme interaction SkM$^*$ turn out to be close to those generated by phenomenological models like those using the proximity potentials. It is also shown that the location and the structure of the fusion barrier in the vicinity of its maximum and beyond can be quite accurately described by a simple analytical form depending only on the masses and the relative isospin of target and projectile nucleus.

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I. INTRODUCTION

The knowledge of the collective potentials between two colliding ions is absolutely crucial for the synthesis of new isotopes. This problem has been the subject of a very active research over the last decade and remains one of the most intensively studied subjects in low-energy nuclear physics in particular in the perspective of the synthesis of super-heavy elements as well as of exotic nuclei far away from the $\beta$-stability line. It has in particular been shown that models based on a macroscopic approach such as the Liquid Drop Model (LDM) or of semi-classical type like the Extended Thomas-Fermi (ETF) method together with the Skyrme energy-density functional are able to reproduce quite accurately experimental data on fission and fusion barriers.

The research concerning the interaction potential between colliding ions goes back to the work of R. Bass (for a review see ref. \cite{Bass:1970}). Since the idea of a proximity potential due to W. J. Świątcecki and coworkers in the late 1970’s \cite{Swiatecki:1977}, many improvements have been proposed to make this phenomenological approach more realistic and general, in particular by taking into account the local curvature of the surfaces of target and projectile \cite{Swiatecki:1977,Swiatecki:1980}. One of the main challenges was, as already mentioned, to give a reliable guideline for the formation and stability of super-heavy elements.

The parameters of the proximity function are usually fitted to experimentally known fusion barriers heights. The basic idea of all proximity models is to determine the potential between the two colliding nuclei as function of the minimal distance $s$ of their surfaces and their so-called reduced radius defined in the case of spherical nuclei as $R = R_1 R_2/(R_1 + R_2)$, where the indices 1 and 2 refer to the target and projectile nucleus respectively.

Experimental data confirm the existence of a pocket in the shape of the nuclear part of the potential. This feature plays an essential role for the formation probability but also for the stability of the compound nucleus in the fusion experiments. Indeed, if the pocket is deep and wide, several quasi-bound states might exist and the probability of forming that compound nucleus is large.

If, on the other hand, this minimum is shallow and narrow no such states will exist. It would therefore be of great help to have at hand a simple, yet sufficiently accurate phenomenological expression for the determination of fusion barriers in order to evaluate the most favorable reaction for the formation of a given compound nucleus.

The aim of our present investigations is to show that the shape of the proximity potential can be, indeed, quite accurately determined through self-consistent semi-classical calculations. We proceed in a way similar to that suggested in Ref. \cite{Swiatecki:1980} and recently used in Ref. \cite{Swiatecki:1999}. After introducing the Skyrme Hartree-Fock energy-density functional together with the semi-classical ETF approximation in Section II we explain in Section III how this approach can be used to calculate fusion barriers. In Section IV the fusion barriers obtained in this way for a sample of 269 different reactions (different combinations of target and projectile) leading a priori to different isotopes of the super-heavy elements with even charge numbers in the range $Z = 108-114$ are presented and compared to the barriers obtained in other theoretical models. Based on these fusion-barrier calculations we present in Section V a simple analytical expression for this potential and show that it is able to reproduce very accurately the fusion barrier heights obtained in the ETF approach. Conclusions are finally drawn in Section VI.

II. THE SKYRME ETF APPROACH TO NUCLEAR STRUCTURE

For the calculation of the interaction potential between the two nuclei we need an energy-density functional which has proven its capacity to correctly describe nuclear ground-state properties. As we are interested in the potential energy resulting from the interaction of the tails of the density distributions of target and projectile, a very precise description of the nuclear surface seems absolutely crucial. The Skyrme effective interaction has been shown to have this property \cite{SkIPI:1980,SkIPII:1980} and has been, together with Gogny’s force \cite{Gogny:1986}, the most successful effective nucleon-nucleon interaction over the last
where the constants \( B_i \) are combinations of the usual Skyrme-force parameters \( t_j \) and \( x_j \). \( \frac{\hbar^2}{2m} \tau_q \) and \( J_q \) designate the kinetic energy density and spin-orbit density of charge state \( q \), \( q = \{ n, p \} \) and non indexed quantities correspond to the sum of neutron and proton densities such as \( \rho = \rho_n + \rho_p \).

Since our aim is to evaluate fusion barriers, a quantity which is essentially determined by the radii and tails of the density distributions of target and projectile, we have chosen the semi-classical approximation known as the Extended Thomas-Fermi (ETF) method \[11\] to determine in a self-consistent way the structure of projectile and target nuclei.

The ETF approach allows to express \( \tau_q \) and \( J_q \) as functions of the local density \( \rho_q \) and its derivatives. This functional expression has the form of an expansion with particle-number and isospin symmetry (as would be the case for rotating nuclei) only even powers of \( \rho \) appear so that the semi-classical expansion of the kinetic energy density will take the form

\[
\tau_q[\rho_q] = \tau_q^{(TF)}[\rho_q] + \tau_q^{(2)}[\rho_q] + \tau_q^{(4)}[\rho_q]; \; q = \{ n, p \} . \tag{2}
\]

At lowest order in the ETF expansion one has the well-known Thomas-Fermi kinetic energy density

\[
\tau_q^{(TF)}[\rho_q] = \frac{3}{5}(\frac{3\pi^2}{2})^{2/3} \rho_q^{5/3} , \tag{3}
\]

whereas the second-order contribution is given by:

\[
\tau_q^{(2)}[\rho_q] = \frac{1}{36} \frac{1}{\rho_q} \frac{\nabla \rho_q}{\rho_q} + \frac{1}{3} \nabla \rho_q \cdot \frac{\nabla f_q}{f_q} + \frac{1}{6} \rho_q \frac{\Delta f_q}{f_q} - \frac{1}{12} \rho_q \left( \frac{\nabla f_q}{f_q} \right)^2 + \frac{1}{2} \left( \frac{2m}{\hbar^2} \right)^2 \rho_q \left( \frac{\Delta f_q}{f_q} \right)^2 . \tag{4}
\]

Here the effective-mass form factor \( f_q = m/m^*(\vec{r}) \), is given by

\[
f_q(\vec{r}) = \frac{m}{m^*(\vec{r})} = \frac{2m}{\hbar^2} \left( \frac{\delta \mathcal{E}(\vec{r})}{\delta \tau_q(\vec{r})} \right) = 1 + \frac{2m}{\hbar^2} [B_3 \rho_q(\vec{r}) + B_4 \rho_q(\vec{r})] \tag{5}
\]

and the spin-orbit potential as

\[
\bar{W}(\vec{r}) = \frac{\delta \mathcal{E}(\vec{r})}{\delta J_q(\vec{r})} = -B_6 \nabla (\rho + \rho_q) . \tag{6}
\]

In the ETF approach one also obtains a semi-classical expansion for the spin-orbit density. Since the spin is a pure quantal phenomenon which does not have any classical analog, the semi-classical expansion of \( \bar{J} \) starts at order \( \hbar^2 \) and the leading term is given by

\[
\bar{J}_q^{(2)} = -\frac{2m}{\hbar^2} \frac{\rho_q}{f_q} \bar{W} . \tag{7}
\]

This now, however, means that one is able to express the total energy density \( \mathcal{E} \) as a unique functional of the proton and neutron density alone and to perform a variational calculation of the ground-state properties of a nucleus, where the variational quantities are \( \rho_n(\vec{r}) \) and \( \rho_p(\vec{r}) \). That such a unique functional must exist for a system of interacting Fermions has been shown by Hohenberg and Kohn \[12\]. In the general case this functional is, however, perfectly unknown. It is the achievement of the ETF approach to derive this functional in the semi-classical limit in a systematic way.ETF variational calculations have indeed proven, when the semi-classical expansion is carried through to order \( \hbar^4 \) \[11\[13\], extremely successful to describe average (liquid-drop type) nuclear properties (see Ref. \[11\] for a review). It has in particular been shown \[11\[14\[15\] that modified Fermi functions of the form

\[
\rho_q(r) = \rho_q^{(0)} \left( 1 + e^{-r - R_q} \right)^{-\gamma_q} \tag{8}
\]

are in that case a very good approximation to the full variational solution. A systematic analysis of the variation of the density parameters \( \rho_q^{(0)} \), \( a_q \) and \( \gamma_q \) (the parameter \( R_q \) is then determined through particle-number conservation) which are the variational parameters of the ETF approach, with the mass number \( A \) and the isospin parameter \( I \) can be found in Ref. \[16\].

We have carried out these kind of 4th order ETF calculations, to determine the structure of target and projectile nucleus. The densities obtained in this way are then used to determine the fusion potential between the two nuclei as will be explained in the following.

### III. THE ETF FUSION POTENTIAL

For evaluating the fusion potential we will use the sudden approximation, i.e. keeping the densities of the colliding ions fixed and neglecting all possible rearrangement effects. At first sight, this looks like a quite crude approximation. For a fusion reaction the beam energy per nucleon is, indeed, quite small as compared to the Fermi
energy and an adiabatic treatment would be more appropriate. One has, however, to keep in mind that the essential characteristics of the fusion barrier, as its structure around the above mentioned pocket, are determined at distances larger and close to the touching configuration. Defining the minimal distance \( s \) between the equivalent sharp surfaces of the liquid drops identifying the two nuclei we see that the essential features of the fusion barrier or cross-sections are determined at the distances \( (s > 0) \), where the sudden approximation seems to be a very reasonable approach. We can then evaluate the nuclear part of the interaction potential \( V_{\text{nuc}} \) of two spherical colliding ions as function of the distance \( d \) between theirs centers of mass (see Fig. 1) as:

\[
V_{\text{nuc}}(d) = \int \left\{ E_{\text{nuc}}[\rho^{(1)}(\vec{r}) + \rho^{(2)}(\vec{r} - \vec{d})] - E_{\text{nuc}}[\rho^{(1)}(\vec{r})] - E_{\text{nuc}}[\rho^{(2)}(\vec{r} - \vec{d})] \right\} d^3r ,
\]

where \( E_{\text{nuc}} \) is the nuclear part of the energy-density, Eq. (4), and \( \rho^{(i)}(\vec{r}) \) denotes the density distribution of nucleus \( i \) alone ((1) labeling e.g. the target and (2) the projectile).

If the distance \( d \) between the two nuclei is much larger than the sum of the half density radii \( (d \gg R_1 + R_2) \) then the nuclear part of the interaction should vanish because of the short range of the nuclear forces:

\[
\lim_{d \to \infty} E_{\text{nuc}} \left[ \rho^{(1)}(\vec{r}) + \rho^{(2)}(\vec{r} - \vec{d}) \right] = E_{\text{nuc}} \left[ \rho^{(1)}(\vec{r}) \right] + E_{\text{nuc}} \left[ \rho^{(2)}(\vec{r}) \right] .
\]

Thus, the nuclear part of the interaction potential (10) between the nuclei is non negligible only when the distance \( s \) between the nuclear surfaces of both nuclei is smaller then a few fm. The Coulomb interaction between the two ions is given as usual in the form

\[
V_{\text{Coul}}(d) = \int \frac{\rho_{\text{ch}}^{(1)}(\vec{r}_1) \rho_{\text{ch}}^{(2)}(\vec{r}_2)}{r_1 - r_2} d^3r_1 d^3r_2
\]

where we simply assume that the charge density is given in terms of the proton density by \( \rho_{\text{ch}}^{(i)} = e \rho_p^{(i)} \) where the latter can be approximated in the ETF approach by Eq. (5).

### IV. FUSION BARRIERS FOR SUPER-HEAVY ELEMENTS

The fusion barrier appears as the result of the competition between the long-range repulsive Coulomb interaction \( V_{\text{Coul}} \) and the short-range attractive nuclear forces \( V_{\text{nuc}} \) as is illustrated on Fig. 2, where the total fusion barrier is plotted as function of the distance \( d \) (see Fig. 1) of the centers of mass of projectile and target nucleus as well as of the distance \( s \) between their half-density surfaces. One notices that for distances \( s \geq 3 \) fm the attractive nuclear part of the fusion potential almost vanishes and the barrier is just determined by the repulsive Coulomb potential. Taking the diffuseness of the charge-density distribution into account reduces the height of the fusion barrier only by about 1 MeV as compared to the barrier obtained with point charge distributions of target and projectile.

![FIG. 2: Shapes of total (nuclear + Coulomb) fusion barriers \( V \) (full line) as function of the center-of-mass distance \( d \) (top) and the distance between the equivalent sharp surfaces \( s \) (bottom) for the reaction \( ^{50}\text{Ti} + ^{238}\text{U} \) leading to the super-heavy element \( Z = 114 \). Also shown are the exact Coulomb barrier (thin line) and the one corresponding to two point charges (dashed line).](image)

It is evident that when the overlap of the densities of the colliding nuclei becomes large, e.g. when \( s \leq 0 \) (dotted line in Fig. 2) the sudden approximation used here becomes more and more questionable. Our aim, however, is not to give a precise description of the entire fusion potential, i.e. also for large negative \( s \) values, but rather to obtain some reasonable estimates of the height \( E_B \) of the fusion barrier. Fig. 3 shows \( E_B \) obtained in the sudden approximation and neglecting deformation effects of the colliding ions for 269 different reactions (with \( \beta \)-stable targets ranging from \(^{168}\text{Er} \) to \(^{238}\text{U} \)) leading to different isotopes of the super-heavy elements with even charge numbers between \( Z = 108 \) and \( Z = 114 \). The barriers shown are the ones obtained with the Skyrme forces SkM* (9) (barriers corresponding to the Skyrme

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*Fig. 1: Definition of target and projectile coordinates.*

*Fig. 2: Shapes of total (nuclear + Coulomb) fusion barriers \( V \) as function of the center-of-mass distance \( d \) (top) and the distance between the equivalent sharp surfaces \( s \) (bottom) for the reaction \( ^{50}\text{Ti} + ^{238}\text{U} \) leading to the super-heavy element \( Z = 114 \). Also shown are the exact Coulomb barrier (thin line) and the one corresponding to two point charges (dashed line).*
FIG. 3: Height of fusion barriers corresponding to the different reactions leading to different isotopes of the S.H. elements with \( Z = 108, 110, 112, 114 \), evaluated in our ETF approach (thick line) and in the proximity model of Ref. [17] (thin lines), as function of the projectile neutron number.

SLy4 interaction are identical to within 1 MeV). The thin lines illustrate the heights of the fusion barriers obtained in the Myers-Świątecki proximity model [17]. Barrier heights evaluated using the prescription of Ref. [18] are very close to the former differing by not more than 2 MeV for all the reactions considered here.

V. A SIMPLE ANALYTICAL FUSION POTENTIAL

The nuclear part of the potential between two colliding ions can be quite well reproduced by the approximate form

\[
V_{\text{nuc}}(d) \approx \tilde{V}_{\text{nuc}}(d) = V_0 e^{-\alpha (d-d_0)^2},
\]

where \( d \) is the distance between the centers of mass of target and projectile and \( d_0 \) the distance for which the nuclear potential has its minimum. \( d_0 \) and the depth \( V_0 \) of the potential are a direct result of our semi-classical calculation. These two quantities are parametrized in the following way as functions of the masses \( A_1, A_2 \) and reduced isospins \( I_i = (A_i - 2Z_i)/A_i \) of target and projectile nuclei

\[
d_0(A_1, A_2) = r_0(A_1^{1/3} + A_2^{1/3}) + b,
\]

and

\[
V_0(A_1, A_2, I_1, I_2) = v_0 \left[1 + \kappa (I_1 + I_2)\right] \frac{A_1^{1/3} A_2^{1/3}}{A_1^{1/3} + A_2^{1/3}},
\]

where the values of the parameters entering into these expressions can be adjusted to the ETF nuclear potentials.

To obtain the potential that the system of two colliding nuclei experiences we have to add the Coulomb potential, Eq. (11), to the nuclear part. For distances large compared to the sum of the equivalent-sharp-surface radii, this Coulomb potential is very well approximated by the Coulomb potential between two point charges, but as soon as the densities of the two nuclei interpenetrate this approximation will no longer give good results and it turns out that the difference

\[
\Delta V_{\text{Coul}}(d) = V_{\text{Coul}}(d) - \frac{Z_1 Z_2 e^2}{d}
\]
will be, in the case of the super-heavy elements considered here, of the order of 3 MeV already in the vicinity of the touching configuration $(s = 0)$.

Instead of calculating the diffuse-surface Coulomb energy explicitly for each reaction under consideration, the idea is to develop an easy-to-use expression to approximate in a reliable way the ETF fusion potential between two nuclei developed above, including the full Coulomb potential. That is why we propose to write this potential in the form

$$
\tilde{V}(d) = \tilde{V}_{\text{nuc}}(d) + \frac{Z_1 Z_2 e^2}{d},
$$

(16)

where the term $\tilde{V}_{\text{nuc}}$, which now contains the Coulomb-energy difference $\Delta V_{\text{Coul}}$, Eq. (15), in addition to the nuclear potential $\tilde{V}_{\text{nuc}}$, is approximated by Eq. (12) with the parameters $d_0$ and $V_0$ being given by Eqs. (18) and (19). It is clear in this context that these new parameters can turn out to take values that could be quite different as compared to those describing the nuclear part alone.

To determine these quantities we perform a simultaneous fit of the 5 free parameters to the fusion potentials of the 269 reactions obtained in the above described ETF approach (see Fig. 3). We proceed in the following way: What we are interested in is primarily the precise description of the location $d_{\text{max}}$ and the height $V_{\text{max}}$ of the total fusion barrier, and we therefore attach a maximum weight to their best possible reproduction. When going to smaller distances, i.e. towards negative values of $s$, the Coulomb-energy difference $\Delta V_{\text{Coul}}$, Eq. (15), grows larger, but also the nuclear potential obtained in our sudden approximation becomes less and less reliable. That is why we attach a decreasing importance to the reproduction of the fusion barriers for smaller and smaller distances. For increasing distances $d > d_{\text{max}}$, on the other hand, both the nuclear potential $V_{\text{nuc}}$ as well as the Coulomb correction $\Delta V_{\text{Coul}}$ go rapidly to zero and our approximation form (16) becomes better and better. We therefore attach again less weight to the precise reproduction of the values with large positive values of $s$. We have thus imagined a least-square-fit procedure with a normalized weight function of Gaussian form and with a width of 1 fm centered at $d = d_{\text{max}}$. The values of the parameters obtained in this way are listed in Table 1.

| $\tau_0$ [fm] | $b$ [fm] | $v_0$ [MeV] | $\kappa$ | $\alpha$ [fm$^{-2}$] |
|----------------|-----------|-------------|----------|-----------------------|
| 1.183          | -2.400    | -46.07      | -0.4734  | 0.173                 |

Tab. 1: Values of parameters entering the fit of the fusion potential, Eq. (16)

The final criterion of the accuracy of our approach consists in its ability to reproduce the height and shape of the fusion barriers for all 269 reactions obtained within the ETF approach with the SkM* Skyrme interaction. The r.m.s. deviation of the exact ETF fusion potential and its approximation by Eq. (16) is only of 0.27 MeV at the top of the barrier and of 0.37 MeV for the touching configuration $(s = 0)$.

Such a fusion barrier is shown on Fig. 4 for the reactions $^{48}$Ca$+^{232}$Th. As one can see, the ETF barrier is almost perfectly reproduced by our analytical expression, Eq. (10) with (12). The barrier height is also almost the same as that obtained in the proximity model of Ref. [17].

[FIG. 4: Fusion barrier for the reaction $^{48}$Ca$+^{232}$Th obtained within the ETF approach (full line), its approximate analytical form, Eq. (10) (dashed line) and the proximity potential of Ref. [17] (dotted line).]

It is obvious from Fig. 3 that the agreement between our ETF approach and the proximity model is not always going to be that close. If one considers e.g. the reaction $^{116}$Cd$+^{154}$Sm one already concludes from Fig. 3 that the barrier heights of the two approaches are going to be different by some 7 MeV (or 2%). One also notices that the minimum obtained in our ETF approach is quite shallow, whereas the proximity potential does not make any predictions about the region $s < 0$. One could now speculate about the validity of our approach close to and inside the touching configuration. The enhancement of the height of the fusion barriers related to the sudden approximation is obviously related to the concept of the diabatic fusion barriers advocated by W. Nörenberg and co-workers [19].

The coincidence of the ETF fusion barrier heights with those obtained in the proximity approach for very asymmetric reactions $(A_1 \gg A_2)$ seems to be related to the value $s_{\text{max}}$ of the distance $s$ of the equivalent sharp surfaces of the two colliding nuclei at the top of fusion barrier, as this is demonstrated on Fig. 5. Comparing Figs. 3 and 5 one can, indeed, observe that the enhancement of the ETF barrier height relative to prediction of the proximity model is larger as the distance of the sharp surfaces of the two nuclei at the top of the barrier gets smaller which is the case for the reactions between nearly symmetric nuclear systems.

As we have just considered fusion reactions leading
predicts fusion barriers that are quite close to the ones obtained with the phenomenological proximity approach of Myers and Świątecki \[\text{(17)}\]. We have given, in addition, an analytical form allowing for a simple approximation of the ETF fusion barriers, thus providing a very simple evaluation of fusion potentials for reactions throughout the periodic table. We believe that such an approach could serve as a guide-line for the research of the synthesis of super-heavy elements.

It is also quite remarkable that our simple phenomenological ansatz, Eq. \[\text{(16)}\], adjusted to the reactions leading to super-heavy elements was able to reproduce even the fusion barrier of very light systems in a quite satisfactory way with a relative error of 2\% at most.

One might also speculate about the importance of deformation on the barrier heights obtained in our approach. It seems immediately evident that taking into account deformation as an additional degree of freedom of the system target-projectile could often lead to a decrease of the fusion barrier \[\text{(20)}\]. One knows, indeed, that e.g. the Coulomb barrier is substantially lower for two nuclei with ellipsoidal deformation and tip-to-tip orientation as compared to a different orientation or in the absence of deformation. It is obvious that for a system like \[^{116}\text{Cd} + ^{154}\text{Sm}\], which we briefly discussed above, where at least the target nucleus shows a substantial deformation, such an effect plays a non negligible role which implies that taking deformation into account in our ETF approach might lead to much lower fusion barriers for those systems.

**VI. CONCLUSIONS**

We have presented a model allowing for a systematic investigation of fusion barriers between heavy nuclei. It has been demonstrated that our approach which is based on a self-consistent semi-classical description of projectile and target nucleus and has no adjustable parameter to the super-heavy elements with even values of \(Z\) between \(Z = 108 - 114\) one might doubt about the utility of such an analysis for the description of fusion barriers in other regions of the atomic chart. We have therefore applied our phenomenological expression to the reactions \[^{160,162,166}\text{Dy} + ^{46-50}\text{Ti}\] as well as to the very light system \[^{48}\text{Ca} + ^{48}\text{Ca}\]. To our great surprise the predictions based uniquely on our knowledge of the ETF barriers of the super-heavy system gave astonishingly good results for these lighter systems with a deviation between ETF results and those of the simple analytical expression, Eq. \[\text{(16)}\], of less than 0.7 MeV for the former and of about 1.3 MeV for the latter system.

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