Energy dependence of nucleus-nucleus potential close to the Coulomb barrier

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The nucleus-nucleus interaction potentials in heavy-ion fusion reactions are extracted from the microscopic time-dependent Hartree-Fock theory for mass symmetric reactions $^{16}\text{O}+^{16}\text{O}$, $^{40}\text{Ca}+^{40}\text{Ca}$, $^{48}\text{Ca}+^{48}\text{Ca}$, and mass asymmetric reactions $^{16}\text{O}+^{40,48}\text{Ca}$, $^{40,48}\text{Ca}+^{16}\text{O}$, $^{16}\text{O}+^{208}\text{Pb}$, $^{40}\text{Ca}+^{90}\text{Zr}$. When the center-of-mass energy is much higher than the Coulomb barrier energy, potentials deduced with the microscopic theory identify with the frozen density approximation. As the center-of-mass energy decreases and approaches the Coulomb barrier, potentials become energy dependent. This dependence signifies dynamical reorganization of internal degrees of freedom and leads to a reduction of the "apparent" barrier felt by the two nuclei during fusion of the order of 2–3\% compared to the frozen density case. Several examples illustrate that the potential landscape changes rapidly when the center-of-mass energy is in the vicinity of the Coulomb barrier energy. The energy dependence is expected to have a significant role on fusion around the Coulomb barrier.

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I. INTRODUCTION

Heavy-ion fusion reactions give important information on dynamical evolution and dissipative phenomena in a quantum many-body system. Macroscopic models\textsuperscript{1, 2, 3, 4, 5} using suitable estimates of nucleus-nucleus potentials\textsuperscript{6, 7, 8, 9, 10, 11, 12}, and then coupled-channels theories\textsuperscript{13, 14, 15} have been widely used to describe the entrance channel of fusion reactions. These models underline that the interplay between nuclear structure and dynamical effects is crucial to properly describe fusion reactions at energies close to the Coulomb barrier. While in general rather successful, these methods have in common several drawbacks. First, nuclear structure and dynamical effects should be treated in a unified framework. Second, important effects should be guessed \textit{a priori}. This has been illustrated recently to understand new high precision measurements at extreme sub-barrier energies\textsuperscript{16, 17, 18, 19, 20}, where different effects like incompressibility\textsuperscript{21}, nucleon exchange\textsuperscript{22}, and the transition from di-nuclear to compound nucleus descriptions\textsuperscript{23} have been invoked to understand experimental observations\textsuperscript{16, 17, 18, 19, 20}. Then, the hypothesis could only be checked \textit{a posteriori}. From this point of view, it is first desired to use theories where both nuclear structure and nuclear dynamics are considered in a unified framework. Second, the use of theories where all the physical effects mentioned above are automatically incorporated can be of particular interest to disentangle different contributions.

Mean-field theories based on Skyrme Energy Density Functional (EDF) provide a rather unique tool to describe nuclear structure and nuclear reactions over the whole nuclear chart. In nuclear reactions, application of the so-called Time-Dependent Hartree-Fock (TDHF), more than 30 years ago\textsuperscript{24, 25, 26, 27, 28, 29, 30}, to heavy-ion fusion reactions was a major step. With the increasing computer power, more and more accurate description of the nuclear reactions has been achieved. Most recent TDHF simulations include the spin-orbit force\textsuperscript{31, 32, 33, 34, 35, 36} and break all the symmetries (plane and axis symmetries generally assumed to speed up calculations). Moreover, all the terms of the Skyrme EDF used in nuclear structure can now be included\textsuperscript{37, 38, 39, 40, 41, 42, 43, 44}. The possibility to perform full three-dimensional calculations and to use effective forces consistent with nuclear structure is crucial to account for the richness of nuclear shapes that are accessed dynamically. In addition, the great interest of dynamical mean-field theories with respect to other methods is that many effects which are known to affect fusion such as dynamical deformation, nucleon exchange, and nuclear incompressibility are automatically incorporated.

The original purpose of the present work was to benchmark the method proposed in Refs.\textsuperscript{24, 32} to obtain nucleus-nucleus potential and one-body dissipation from the microscopic TDHF dynamics. The possibility to obtain such a potential from a mean-field theory has been studied in several works using the static EDF technique\textsuperscript{45, 46, 47, 48}. More recently, a method called density-constrained TDHF (DC-TDHF)\textsuperscript{49}, which combines TDHF dynamics with minimization technique under constraints on the one-body density, has been applied in Refs.\textsuperscript{41, 42}, the latter being able to incorporate possible dynamical effects through the use of realistic density profiles obtained during the evolution.

Here, we consider a different approach based on a macroscopic reduction of the mean-field dynamics, called hereafter Dissipative-Dynamics TDHF (DD-TDHF). This technique could \textit{a priori} give access not only to nucleus-nucleus potential but also to friction co-

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II. NUCLEUS-NUCLEUS POTENTIAL FROM MICROSCOPIC MEAN-FIELD MODEL

In this section, the extraction of nucleus-nucleus interaction potentials from mean-field theories is discussed. In macroscopic models, these potentials are generally displayed as a function of a few macroscopic collective degrees of freedom describing, e.g., the relative distance, shapes of nuclei, mass asymmetry. Here, we will concentrate on head-on collisions between initially spherical nuclei and assume that the collective space simply identifies with the relative distance $R$ between colliding nuclei. The validity of this approximation in the TDHF context will be discussed below. In the following, we first present a general discussion on different methods to extract nucleus-nucleus potential from a mean-field theory.

A. Some remarks on EDF

The basic ingredient of a nuclear mean-field model is the energy functional of the one-body density $\hat{\rho}$ denoted by $\mathcal{E}[\hat{\rho}]$. In the nuclear context, $\mathcal{E}[\hat{\rho}]$ is expressed in terms of a few parameters generally related to the associated effective interaction. Here, we will use the Skyrme EDF with the SLy4d parameters. This choice is particularly suited to dynamical calculations because of the removal of center-of-mass corrections in the fitting procedure of the force parameters. In the EDF context, static properties of nuclei are deduced by minimizing the functional with respect to all possible one-body densities. The great interest of EDF theory is that the initial complicated many-body problem is replaced by an independent particle problem. Indeed, the minimization procedure is equivalent to find the set of single-particle states that diagonalizes both the self-consistent mean-field defined through the relation $h[\hat{\rho}]_{ij} = \partial \mathcal{E}[\hat{\rho}] / \partial \rho_{ij}$ and the one-body density. At the minimum, we have $[\hat{h}[\hat{\rho}], \hat{\rho}] = 0$.

B. Illustration of fusion with time-dependent EDF

The static EDF theory has also its dynamical counterpart, called time-dependent EDF where the dynamical evolution of nuclear systems is replaced by the one-body density evolution, i.e.,

$$i\hbar \frac{d\hat{\rho}}{dt} = [\hat{h}[\hat{\rho}], \hat{\rho}] = \frac{\partial \mathcal{E}[\hat{\rho}]}{\partial \rho_{ji}} \rho_{ij}.$$

Dynamical calculations presented in this paper are performed with the three-dimensional TDHF code developed by P. Bonche and coworkers with the SLy4d Skyrme effective force. As the initial conditions for the TDHF time evolution, we prepare the density of colliding nuclei by solving static HF equations with the same effective force as the one used in the TDHF. The step size in the coordinate space is 0.8 fm. Then, we calculate the time evolution of the colliding nuclei in the three-dimensional mesh. The time step is 0.45 fm/c and the initial distance is set between 16 – 22.4 fm, depending on reaction. We assume that the colliding nuclei follow the Rutherford trajectory before they reach the initial distance for TDHF. Thus, the initial positions and the momenta of the colliding nuclei are determined. As an illustration, the density evolution of the $^{16}O + ^{208}Pb$ head-on collision at center-of-mass energy $E_{c.m.} = 120$ MeV are shown at three different relative distances in Fig. II.

C. Discussion of nucleus-nucleus potentials deduced from mean-field theories

A good estimate of the interaction potentials felt by the two nuclei in the approaching phase within the EDF theory could be obtained assuming that the densities of the target and projectile remain constant and equal to their respective ground state densities. This leads to the

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1 Note that during the reaction nuclei might be deformed.

2 Although this theory has been called improperly TDHF in the past, we will continue to use this acronym in this work.
so-called *Frozen Density* (FD) approximation (see for instance Ref. [14]). In this limit, the interaction potential between a target and projectile with their ground state densities respectively denoted by $\hat{\rho}_T$ and $\hat{\rho}_P$ reads

$$V^{FD}(R) = E[\hat{\rho}_{PT}](R) - E[\hat{\rho}_T] - E[\hat{\rho}_P],$$

where $\hat{\rho}_{PT} = \hat{\rho}_P + \hat{\rho}_T$ is the total density obtained by summing the densities of the target and projectile assuming that their centers of mass are at a given relative distance $R$. Note that $E[\hat{\rho}_{PT}]$ here neglects the Pauli effect by the two overlapping densities. As we will see the following, we use the property of the extracted potentials with FD technique essentially at the Coulomb barrier. At this point, overlap of the two densities is small and Pauli effect is expected to be accordingly small. It should however be kept in mind that a proper account of the Pauli principle would lead to an increase of the potential for small relative distances.

### D. Matching TDHF with a two-body collision problem

The FD approximation is expected to break down if strong reorganization of internal one-body degrees of freedom occurs in the approaching phase. In the following, methods to extract nucleus-nucleus potential directly from TDHF without assuming frozen densities are discussed.

#### 1. Definition of the separation plane

The first step is to properly define the collective coordinate $R$ that separates the two sub-systems. Here, we follow macroscopic models and define the plane of separation at the neck position. In practice, the neck position is obtained by considering the two densities

$$\rho_{T/P}(r, t) = \sum_{n \in T/P} |\varphi_n^{T/P}(r, t)|^2,$$

where $\varphi_n^{T}(r, t)$ (resp. $\varphi_n^{P}(r, t)$) denote single-particle wave functions initially in the target (resp. projectile) which are propagated in the mean-field of the composite system up to time $t$. Note that, if the approaching phase is fast enough, these densities have no time to evolve and is expected to be very close to their respective ground state densities. The separation plane at a given time $t$ is then defined at the position where iso-contours of the two densities $\rho_T(\mathbf{r}, t)$ and $\rho_P(\mathbf{r}, t)$ cross. An example of densities $\rho_{T,P}(\mathbf{r})$ (solid lines) as well as the deduced separation plane (vertical thick line) is given for the reaction $^{16}\text{O}+^{208}\text{Pb}$ in bottom of Fig. 1. This figure illustrates that the separation plane corresponds to the geometrical neck as generally defined in leptodermous systems.

#### 2. Two-body kinematics

Once the separation plane is defined, all quantities relative to the dynamics of the two sub-systems can be calculated. We associate to each sub-space an index $i = 1, 2$ and a density $\hat{\rho}_i(t)$, which equals the total density in the sub-space "i" and cancels out in the opposite side of the separation plane. Then, all quantities of interest could be computed like the number of nucleons in each side of the separation plane, i.e., $A_i(t) \equiv \text{Tr}(\hat{\rho}_i(t))$. Since we are considering head-on collisions along $x$-axis, the center-of-mass coordinate $R_i(t)$ and associated momentum $P_i(t)$ express as

$$R_i(t) \equiv \text{Tr}(\hat{\rho}_i(t))/A_i(t), \quad P_i(t) \equiv \text{Tr}(\hat{\rho}_i \dot{\hat{\rho}}_i(t)).$$

We can also compute the inertial mass of the two sub-systems, denoted by $m_i$, from the TDHF evolution using $m_i = P_i/R_i$. Once these quantities are obtained, the TDHF dynamics can be reduced to the two-body collision problem where the relative distance $R(t) = R_1 - R_2$, associated momentum $P(t) = (m_2 P_1 - m_1 P_2)/(m_1 + m_2)$, and reduced mass

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

are computed at each time step. Note that, when the two nuclei are far from each other, the reduced mass properly identifies with its initial value $\mu_{ini} = m_A T A_P/(A_T + A_P)$, where $A_T$ and $A_P$ denote respectively the initial target mass number.
the potential is then given by

\begin{align}
\rho & = (\varrho, \gamma) \text{ and projectile mass}^3 \text{ and } m \text{ is the nucleon mass. It is worth mentioning that, while for symmetric reactions } \\
\mu & \text{ remains constant during the collision, for asymmetric case } \mu \text{ may vary after the contact, i.e., } \mu = \mu(R). \text{ The critical discussion on the possible influence of this variation on extracted potentials is presented in Sec. III E.}
\end{align}

E. Dynamical effects on nucleus-nucleus potentials

The great interest of the DC-TDHF method lies in the possibility to access the adiabatic potential accounting for possible evolution of the density along the TDHF path, the so-called density-constrained TDHF (DC-TDHF) technique has been developed. In this method, at each time-step, the density \( \rho(r,t) \) is deduced from TDHF. Then, the EDF is minimized under the constraint that the total density matches \( \rho(r,t) \). Denoting the minimized EDF by \( E_{DC}[\rho(t)](R) \), the potential is then given by

\begin{equation}
V^{DC}(R) = E_{DC}[\rho(t)](R) - E[\dot{\rho}_T] - E[\dot{\rho}_P]. \tag{5}
\end{equation}

The great interest of the DC-TDHF method lies in the possibility to access the adiabatic potential which account for possible dynamical effects and to get information on dissipative process from a fully microscopic theory. In the following, we show that this method is a valuable tool.

1. Discussion on the R-dependent mass

Before presenting applications, additional remarks on the origin of the \( \frac{d\mu(R)}{dR} \) term in Eq. (6) are mandatory. To obtain the equation, we implicitly assumed that the total energy can be written as a sum of a Hamiltonian part and a dissipative part \( E_{\text{diss}} \), i.e.

\begin{equation}
E = \frac{P^2}{2\mu(R)} + V^{DD}(R) + E_{\text{diss}}, \tag{7}
\end{equation}

where the reduced mass depends explicitly on \( R \). For canonical variables \( (R, P) \), the Hamilton part in Eq. (6) arises from the derivative of the kinetic and \( V^{DD} \) part in previous equation. Using \( \frac{1}{2} \frac{d\mu(R)}{dR} \dot{R}^2 = -\frac{d\mu(R)}{dR} \left( \frac{d^2}{dR^2} \right) \), we finally obtain the second equation in (6). The appearance of the R-dependent reduced mass in dynamical mean-field calculations has been reported in Ref. 33, 42 and turned out to be weak before the Coulomb barrier. In all applications presented below we explicitly neglected the second term in the evolution of \( P \). Indeed, including it or not or taking directly \( \mu(R) = \mu_{\text{ini}} \) has no effect on the barrier height and position presented in this work. For the sake of completeness this aspect is illustrated in Sec. III E.

F. Matching TDHF with binary dissipative collisions

An alternative technique proposed in Ref. 29, preliminary tested in Ref. 33, consists in assuming that the time evolution of \( R \) and its canonical momentum \( P \) obey a classical equation of motion including a friction term which depends on the velocity \( \dot{R} \):

\begin{align}
\frac{dR}{dt} & = \frac{P}{\mu(R)}, \\
\frac{dP}{dt} & = -dV^{DD} + \frac{1}{2} \frac{d\mu(R)}{dR} \dot{R}^2 - \gamma(R) \dot{R}, \tag{6}
\end{align}

where \( V^{DD}(R) \) and \( \gamma(R) \) denote respectively the nucleus-nucleus potential and friction coefficient (here "DD" stands for Dissipative Dynamics). The friction coefficient \( \gamma(R) \) describes the effect of energy dissipation from the macroscopic degrees of freedom to the microscopic ones. The great interest of this method is the possibility to access interaction potentials which account for possible dynamical effects and to get information on dissipative process from a fully microscopic theory. In the following, we show that this method is a valuable tool.

III. APPLICATION

A. Procedure to obtain \( V^{DD}(R) \) and \( \gamma(R) \)

In Eq. (6), we have three unknown quantities: the reduced mass \( \mu(R) \) entering in the first equation, the friction coefficient \( \gamma(R) \) and the nucleus-nucleus potential \( V^{DD}(R) \) appearing in the relative momentum evolution. The reduced mass can be directly deduced from a single TDHF trajectory. Indeed, both \( R(t) \) and \( P(t) \) can be computed at all time along the mean-field trajectory. From \( R(t) \), \( \dot{R}(t) \) is simply computed from

\begin{equation}
\dot{R}(t) \equiv \frac{R(t + \Delta t) - R(t - \Delta t)}{2\Delta t} \tag{8}
\end{equation}

where \( \Delta t \) corresponds to the numerical time step used in TDHF. We finally deduced \( \mu(R) \) from \( P(t)/\dot{R}(t) \).

To obtain the two remaining unknown quantities \( \gamma(R) \) and \( V^{DD}(R) \), a single TDHF trajectory is not sufficient.
We assume that the potential energy and the friction parameter are not affected by a slight change in center-of-mass energy and consider two head-on collisions with energies \( E_l = E_{c.m.} \) and \( E_I = E_{c.m.} + \Delta E \) (in practice \( \Delta E / E_{c.m.} \approx 1 - 2% \) is used). A couple of canonical variables \((R_{II}, \dot{R}_{II})\) is associated to each trajectory. Assuming that Eq. (6) applies in both cases with the same potential and friction, we deduce

\[
\gamma(R) = -\frac{\dot{R}_{II}R_{II} = R - [R_{II}]_{R_{II} = R}}{[R_{II}]_{R_{II} = R} - [R_{II}]_{R_{II} = R}}.
\]  (9)

Then, using one of the trajectories, we obtain \( dV^{DD}/dR \) as a function of relative distance. The potential \( V^{DD}(R) \) is deduced by integration over \( R \) using its asymptotic Coulomb potential at large relative distances. The present method clearly relies on the hypothesis that the mean-field dynamics could properly be reduced to a one-dimensional macroscopic description. As we will see, this potential compares rather well with other techniques validating \textit{a posteriori} the macroscopic reduction used in this work. Finally, \( V^{DD}(R) \) is also expected to contain dynamical effects like density evolution.

**B. Illustrative example: \(^{16}\text{O}+^{16}\text{O}\)**

![Graph](image)

**FIG. 2**: Comparison of potential energies for the \(^{16}\text{O}+^{16}\text{O}\) reaction obtained from different models. The solid, dashed, and filled circles-dotted line correspond to the DD-TDHF, DC-TDHF \(^{[41]}\), and FD potentials, respectively. A zoom on the Coulomb barrier region is also shown in the insert.

The potential \( V^{DD}(R) \) obtained with the dissipative dynamics reduction method for the \(^{16}\text{O}+^{16}\text{O}\) reaction at \( E_{c.m.} = 34 \text{ MeV} \) (and \( \Delta E = 1 \text{ MeV} \)) is displayed (solid line) in Fig 2. The DC-TDHF (dashed line) potential obtained in Ref. \(^{[41]}\) and the FD potential (filled circles-dotted line) are also displayed for comparison. Figure 2 shows that potentials extracted from the DD- and DC-TDHF methods are very close from each other (almost identical) even well inside the Coulomb barrier (up to \( R = 5.3 \text{ fm} \)). The fact that the potential deduced from our method matches the DC-TDHF result gives confidence in the specific macroscopic equation (Eq. \( \text{[6]} \)) retained to reduce the microscopic dynamics. In addition, both methods are almost identical to the FD description (for \( R \geq 6.5 \text{ fm} \)). This indicates that little reorganization of densities occurs in the approaching phase. This is indeed confirmed in Fig. 3 where the TDHF density profiles obtained at different relative distances (Left) are directly compared to densities used in the FD approximation for the same \( R \) (Right). At and below the estimated barrier radius \( R_B = 8.46 \text{ fm} \), little difference between the densities \( \rho_{P/T}(X,0,0) \) (Left-solid line) and the ground state densities (Right-solid lines) can be seen. As a consequence, the Coulomb barrier predicted by TDHF is almost identical to the one obtained in the FD case (the difference being less than 0.1 MeV). It is worth mentioning at that point that our method assumes neither sudden nor adiabatic approximation. Last, another conclusion that could be drawn from the matching between DD-TDHF or DC-TDHF and the FD approximation is that Pauli blocking effects which are automatically incorporated in the two former approaches and partially neglected in \( V^{FD} \) do not seem to play a significant role close to the Coulomb barrier in \(^{16}\text{O}+^{16}\text{O}\).

\(^{4}\) Note, however, that a different set of parameters was used for the Skyrme effective interaction and numerical aspects.
FIG. 3: Left: Density profiles $\rho(X,0,0)$ (dashed) and $\rho_{P/T}(t)$ (solid lines) obtained with TDHF for the head-on $^{16}\text{O}+^{16}\text{O}$ collision at $E_{\text{c.m.}} = 34$ MeV at three different times. Each value of relative distance $R$ is indicated in each left panel. Right: Densities $\rho(X,0,0)$ (dashed lines) obtained at the same relative distances within the FD approximation are shown. In this case, $\rho_{P/T}(X,0,0)$ (solid lines) identify with the ground state densities of the $^{16}\text{O}$ nucleus.

Figure 2 indicates that dynamical effects affect marginally the potential felt by the two partners in the approaching phase. In the next section, we will indeed see that similar conclusions hold in most cases studied when $E_{\text{c.m.}}$ is well above the Coulomb barrier. This is the case presented here where $E_{\text{c.m.}}$ is three times more than the Coulomb barrier. In this limit, the spatial organization of nucleons inside each nucleus is almost frozen before the contact.

C. Systematic study of nucleus-nucleus potential at high center-of-mass energy

Previous study is extended to fusion reactions with various combinations of nuclei. Since deformed nuclei have orientations with respect to the collision axis, which increases macroscopic degrees of freedom to be considered, we concentrate on collisions involving spherical nuclei. The DD-TDHF technique is applied to the systems $^{40}\text{Ca}+^{40}\text{Ca}$, $^{48}\text{Ca}+^{48}\text{Ca}$ for mass symmetric reactions and $^{16}\text{O}+^{40,48}\text{Ca}$, $^{40}\text{Ca}+^{48}\text{Ca}$, $^{16}\text{O}+^{208}\text{Pb}$, $^{40}\text{Ca}+^{90}\text{Zr}$ for mass asymmetric reactions.

In all systems, we do expect that, when center-of-mass energy increases, the potential will identify with the FD case. We have checked that this is indeed the case and identifies the minimum energy for which the FD limit is reached. Potentials obtained with the DD-TDHF are displayed by the solid lines in Fig. 4 and are systematically compared with the FD approximation. In Figs. 4(a) and 4(b), the center-of-mass energy used to perform the macroscopic reduction is about two times the Coulomb barrier energy. Similarly to the $^{16}\text{O}+^{16}\text{O}$ reaction case, all the examples presented in Figs. 4(a) and 4(b) follow closely the FD approximation. Higher center-of-mass energies have to be used to reach the FD case in the systems presented in Figs. 4(c) and 4(d). We report in Fig. 5 the center-of-mass energy threshold, denoted by $E_{\text{c.m.}}^{FD}$, which corresponds to the minimal $E_{\text{c.m.}}$ for which the DD-TDHF method gives the FD results (within 5% in general) as a function of the FD barrier. The different Coulomb barrier energies deduced from the DD-TDHF method applied at high center-of-mass energies (denoted by $V_{B}^{DD}$ (high $E_{\text{c.m.}}$)) are reported in Table I. These barriers are systematically compared with the FD case and experimental data taken from Refs. [13, 58, 59]. Overall, we see that the DD-TDHF method applied at high center-of-mass energy gives a qualitative agreement with experiments. It is however noticeable that the barrier height is systematically higher than the experimental observation and that the discrepancy increases as $Z_{P}Z_{T}$ increases.

We will see in the following that part of the difference observed could be understood in terms of departure from the FD limit as the center-of-mass energy approaches the Coulomb barrier. Indeed, as the energy decreases, densities have more time to reorganize.
TABLE I: Energy and radii of the Coulomb barrier extracted from the DD-TDHF method. Here, $V_B^{DD}$ (high $E_{c.m.}$) refers to barrier deduced for $E_{c.m.} > E_{c.m.}^{FD}$, while $V_B^{DD}$ (low $E_{c.m.}$) corresponds to the lowest Coulomb barrier deduced from TDHF using $E_{c.m.} \approx V_B^{FD}$. The experimental values taken from Refs. [13, 58, 59] are reported when available.

| Reaction | $V_B^{DD}$ (MeV) | $V_B^{DD}$ (MeV) | $V_B^{DD}$ (MeV) | $R_B^{DD}$ (fm) | $R_B^{DD}$ (fm) | $R_B^{DD}$ (fm) | $R_B^{DD}$ (fm) |
|----------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| $^{40}$Ca+$^{40}$Ca | 54.7 | 54.54 | 53.35 | 52.8 [58] | 9.8 | 9.2 | 9.82 |
| $^{40}$Ca+$^{40}$Ca | 53.8 | 53.24 | 52.13 | 52.00 [58] | 10.1 | 9.18 | 10.50 |
| $^{40}$Ca+$^{40}$Ca | 52.4 | 52.13 | 50.97 | 51.49 [58] | 10.3 | 9.50 | 10.21 |
| $^{16}$O+$^{208}$Pb | 76.0 | 75.91 | 74.51 | 74.52 [58] | 11.8 | 11.74 | 11.31 |
| $^{40}$Ca+$^{90}$Zr | 99.8 | 99.98 | 97.71 | 96.88 [58] | 10.8 | 10.63 | 11.27 |

D. Center-of-mass energy dependence of nucleus-nucleus potential close to the Coulomb barrier

In the previous examples, we have determined the typical center-of-mass energy above which the potential deduced from the DD-TDHF technique corresponds to the FD case. Here, we show that the extracted potential energy is slightly modified as the center-of-mass energy decreases and approaches the Coulomb barrier. As shown below, this energy dependence of the nucleus-nucleus potentials underlines the role of dynamical effects.

1. Dynamical reduction of the Coulomb barrier energy

To illustrate the center-of-mass energy dependence of the potential, Figure 6 presents potentials obtained with the DD-TDHF method using several center-of-mass energies ranging from $E_{c.m.} = 55$ MeV to 100 MeV for the $^{40}$Ca+$^{40}$Ca reaction. Again, in the high energy limit, potentials identify with the FD case. In addition, an increase of center-of-mass energy from $E_{c.m.} = 90$ to 100 MeV leads to identical results indicating the stability of the method as the energy increases. In opposite, as $E_{c.m.}$ decreases, potentials deduced from the DD-TDHF deviates from the FD case. As $E_{c.m.}$ approaches the Coulomb barrier energy, a small change in $E_{c.m.}$ significantly affects $V_B^{DD}$ as illustrated by the two energies $E_{c.m.} = 55$ MeV and 57 MeV displayed in Fig. 6. In order to quantify this dependence, we have reported in Fig. 7 values of the Coulomb barrier, denoted by $V_B^{DD}$, deduced from the DD-TDHF method as a function of center-of-mass energy. Again, if $E_{c.m.}$ is high, $V_B^{DD}$ becomes very close to the FD case. As $E_{c.m.}$ decreases, $V_B^{DD}$ is more and more reduced compared to $V_B^{FD}$. This effect, observed in all the cases considered here and called hereafter "dynamical barrier reduction", is a direct consequence of reorganization of densities in the approaching phase. This is clearly illustrated in Fig. 8 where density profiles obtained for the $^{40}$Ca+$^{40}$Ca reaction at three center-of-mass energies ($E_{c.m.} = 55, 57$, and 90 MeV are shown from top to bottom respectively) and for specific $R$ values. In Fig. 8 only the case of $E_{c.m.} = 90$ MeV resembles the FD case. At lower energies, a clear de-
variation from the FD density profile is observed. Considering \( E_{c.m.} = 55 \) MeV, as the two partners approach deformation of the two nuclei takes place. This deformation initiates the formation of a neck at larger relative distances compared to \( E_{c.m.} = 90 \) MeV. The center-of-mass energy dependence of potential extracted with the DD-TDHF technique reflects the difference in the density profiles accessed dynamically during the mean-field evolution. Note that similar dependence is \textit{a priori} also expected in the DC-TDHF method \cite{41, 42} which accounts for the dynamical deformation of the densities.

![Density profiles obtained in TDHF for different relative distances](image)

FIG. 8: Density profiles obtained in TDHF for different relative distances \( R = 10.26 \) (left), 9.82 (middle), and 9.52 fm (right) for the \( ^{40}\text{Ca} + ^{40}\text{Ca} \) reaction at three different center-of-mass energies: \( E_{c.m.} = 55, 57, \) and 90 MeV from top to bottom. These energies corresponds to those used in Fig. 7 to obtain \( V^{DD}(R) \).

In all cases considered in this work, a reduction of the "apparent" Coulomb barrier seen by the two nuclei before fusion is observed compared to the FD case. This reduction could always be assigned to large density deformation close to the barrier. In order to quantify the magnitude of the dynamical reduction effect, we have systematically extracted the lowest barrier energy. This quantity (denoted by \( V_B^{DD} \) (low \( E_{c.m.} \))), reported in the third column of Table 1 is obtained when the center-of-mass energy used in DD-TDHF equals the corresponding \( V_B^{FD} \). In Fig. 9, the difference between the lowest barrier and the FD barrier is displayed as a function of \( V_B^{FD} \). We see that the difference increases almost linearly with \( V_B^{FD} \), i.e., with the initial \( Z_P Z_T \). As mentioned previously, the Coulomb barrier energy obtained within the FD approximation generally overestimates the Coulomb barrier energy deduced from experiments (see Table 1). The discrepancy increases as \( Z_P Z_T \) increases. Interestingly enough, the lowest energy \( V_B^{DD} \) is much closer to the experimental observation in particular for large \( Z_P Z_T \).

![Difference between barrier and lowest barrier](image)

FIG. 9: Difference between the barrier obtained with the FD approximation and the lowest barrier with DD-TDHF as a function of \( V_B^{FD} \). In practice, the lowest barrier is obtained by using center-of-mass energy at or close to \( V_B^{FD} \).

2. Critical discussion on the one-dimensional reduction: The \( ^{16}\text{O} + ^{208}\text{Pb} \) case

Previous discussions point out that various density profiles might be accessed depending on the center-of-mass energy used in TDHF. In macroscopic models, such a diversity in densities is usually accounted for by considering multidimensional collective space where deformation and/or neck are explicitly treated as relevant variables \cite{1, 2, 3, 4, 5}. Therefore, the energy dependence of the potential deduced with the DD-TDHF method should \textit{a priori} be understood as different paths in a more complex multidimensional potential energy landscape. As a consequence, one should also \textit{a priori} consider macroscopic reduction of TDHF with additional collective degrees of freedom which might become extremely complicated.

Here, we show that the simple one-dimensional macroscopic reduction still contains meaningful information on the fusion process. We consider the \( ^{16}\text{O} + ^{208}\text{Pb} \) reaction for which extensive TDHF calculations have been performed \cite{39, 50}.

Different potentials deduced for this reaction using the DD-TDHF method with different center-of-mass energies are displayed in Fig. 10. A more complex energy dependence is observed in this case compared with the \( ^{40}\text{Ca} + ^{40}\text{Ca} \) reaction displayed in Fig. 6. In particular at intermediate center-of-mass energies (100 MeV < \( E_{c.m.} \) < 200 MeV), the nucleus-nucleus potential is above the FD case. This is clearly illustrated in Fig. 11 where the Coulomb barrier energy \( V_B^{DD} \) is shown as a function of \( E_{c.m.} \). A bump for intermediate center-of-mass energies is clearly seen. Note that a similar behavior is also observed in the \( ^{40}\text{Ca} + ^{90}\text{Zr} \) case indicating that the energy dependence might be more complex as \( Z_P Z_T \) increases. However, in view of the potential change compared to the center-of-mass energy involved (almost two
times $V_{F^D}$ this bump is not expected to change drastically the fusion probability obtained with TDHF. On opposite, when the center-of-mass energy is close to the Coulomb barrier, a small change in the potential will modify significantly the fusion probability. In the following, we will concentrate on this region.

The low energy fusion TDHF threshold which is defined as the minimal center-of-mass energy required to fusion in TDHF is also presented as an arrow in Fig. 11. A very precise value of this threshold has been obtained in Ref. [36] using the same TDHF code with the SLy4d Skyrme effective interaction by performing a large number of TDHF calculations and was found to be 74.45 MeV. The lowest barrier energy obtained with the DD-TDHF method perfectly matches this threshold. Again, this gives additional confidence in this method to provide precise information on nucleus-nucleus potential extracted.

### E. Effect of coordinate-dependent mass

In previous sections, the macroscopic equation (6) with neglecting the term $\frac{1}{2} \frac{d\mu(R)}{dR} \dot{R}^2$ is used as a starting point to extract potentials from the DD-TDHF method. This equation is a priori only valid for systems with constant reduced mass. This condition is exactly fulfilled by the mean-field evolution for symmetric collisions. For asymmetric reactions, dependence of the reduced mass with relative distance is possible. This situation is illustrated in Fig. 12 where the reduced mass estimated through Eq. (8) divided by its initial value $\mu_{ini}$ is shown as a function of $R/R_{FB}$. In all cases, a deviation from the initial value is observed. In particular, this deviation might be significant for the most asymmetric case $^{16}$O+$^{208}$Pb at small relative distances. Similar behavior has been discussed in Ref. [42]. In all cases, the center-of-mass energy used in the calculation corresponds to $V_{F^D}$ (see table I).

To estimate the possible effect of the $R$-dependent reduced mass on the extracted potential and friction coefficient, we also extracted potentials and friction coefficients from Eq. (8) including the term $\frac{1}{2} \frac{d\mu(R)}{dR} \dot{R}^2$. Using the same procedure as described in Sec. IIIA a new potential $V_{DD}$ can be extracted. In Fig. 13 potentials with (solid lines) and without (filled triangles) this term are compared for the mass-asymmetric $^{16}$O+$^{40}$Ca,
automatically incorporate dynamical effects during the approaching phase which could be traced back in the energy dependence of the nucleus-nucleus potential. This energy dependence has been systematically investigated for the mass symmetric reactions $^{16}\text{O}+^{16}\text{O}$, $^{40}\text{Ca}+^{40}\text{Ca}$, $^{48}\text{Ca}+^{48}\text{Ca}$ and mass asymmetric systems $^{16}\text{O}+^{40,48}\text{Ca}$, $^{16}\text{O}+^{208}\text{Pb}$, $^{40}\text{Ca}+^{48}\text{Ca}$, $^{40}\text{Ca}+^{90}\text{Zr}$. For this systematic, the following aspects have been discussed:

- We show that in all reactions the minimal energy ($E_{c.m.}^D$) for which the FD potential is recovered with the DD-TDHF can always be identified. This energy has been systematically investigated. We have shown, that $E_{c.m.}^F/E_{c.m.}^D$ increases as the $Z_T Z_T$ increases (Fig. 13).

- A clear energy dependence of extracted potential, due to dynamical effects which modify density profile, has been observed in all cases. For systems with $Z_T Z_T \leq 400$ a continuous decrease of the apparent Coulomb barrier is seen as the center-of-mass energy decreases (Fig. 7) while in other systems ($^{16}\text{O}+^{208}\text{Pb}$ and $^{40}\text{Ca}+^{90}\text{Zr}$) more complex energy dependence of the Coulomb barrier energy is obtained (Fig. 11).

- In all cases, nucleus-nucleus potential deduced from the DD-TDHF method varies rapidly as the center-of-mass energy approaches the Coulomb barrier energy. Such a rapid change could be assigned to the difference in density profiles dynamically obtained in various TDHF calculations performed with slightly different $E_{c.m.}$.

- Dynamical effects induce a reduction of the apparent barrier compared to the FD case of the order 2–3% of $V_B^{FD}$ (Fig. 8). While the FD Coulomb barrier generally overestimates the Coulomb barrier estimated experimentally, barriers including the dynamical reduction effect become very close to the experimental case (Table 1).
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