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Elimination of fast variables and initial slip: a new mechanism to the fusion hindrance in heavy-ion collisions

David Boilley

GANIL, CEA/DRF-CNRS/IN2P3, BP 55027, F-14076 Caen cedex 5, France
Normandie Univ, UNICAEN, Caen, France

E-mail: boilley@ganil.fr

Yasuhisa Abe

Research centre for Nuclear Physics (RCNP), Osaka University, 10-1 Mihogaoka,
Ibaraki, 567-0047 Osaka, Japan

Bartholomé Cauchois

GANIL, CEA/DRF-CNRS/IN2P3, BP 55027, F-14076 Caen cedex 5, France
Normandie Univ, UNICAEN, Caen, France

Caiwan Shen

School of Science, Huzhou University, Huzhou, 313000 Zhejiang, People's
Republic of China

Abstract. Synthesis of superheavy elements by fusion-evaporation reactions is limited by the extremely low cross-sections. One of the reasons of the reduced cross-sections is the so-called quasifission that hinders fusion for reactions with heavy systems. It is well acknowledged that fusion hindrance is due to a conditional saddle that has to be overcome in a dissipative environment to reach the compound configuration from the contact point. However, the dynamical description is not yet well established. In this communication we show that elimination of fast variables to reduce the number of degrees of freedom leads to a slip of the initial conditions of the slow variables which has a significant impact on the amplitude of the hindrance phenomenon. The energy dependence of the slip is similar to phenomenological shift introduced in the “fusion by diffusion” model.

Keywords: superheavy elements, reaction dynamics, fast variables elimination
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1. Introduction

Finding the limit of existence of nuclei is one of the challenging research programs in nuclear physics. The size of the nuclei is limited by the fission barrier that vanishes around the atomic charge $Z = 100$ within the Liquid Drop Model. Beyond, nuclei only owe their existence to the extra-stability provided by the shell correction energy. They form the so-called superheavy elements. Their synthesis is a challenge due to the extremely low cross-sections, at the order of the picobarn for the heaviest elements produced by fusion-evaporation reactions. The reasons are twofold: first, with low fission barriers, most of the compound nuclei formed during the reaction undergo fission instead of cooling down through neutron evaporation. Second, the fusion process is hindered compared to reactions with lighter nuclei.

A correct description of the hindrance mechanism is necessary to improve the predictive power of models describing the whole reaction leading to the synthesis of superheavy elements. However, as pointed out by few comparisons [1, 2, 3], there are still large discrepancies between models and a small change in the cross-sections could mean months of beam time.

The first predictions of fusion-evaporation cross-section were far too optimistic [4]. Nix and Sierk showed that the dynamical trajectory for the fusing system must overcome a conditional saddle in a multidimensional space to form a compound nucleus. In contrast to light systems, the conditional saddle point lies inside the point of hard contact in heavy-ion reactions [5]. To emphasise the role of this barrier, their results were presented with zero dissipation and lead to the so-called extra-push energy concept.

Later, Świątecki [6, 7] introduced a dynamical model that emphasises the role of rapid dynamical deformations away from the configuration of two spheres in contact. It also includes dissipation that leads to the requirement of even higher energies to fuse. Soon, experimental evidences confirmed the model [8, 9, 10] and several calculations tried to estimate the reduction of the cross-section due to fusion hindrance [11, 12]. For a review, see Ref. [13].

Although dissipation plays a crucial role in understanding the fusion hindrance [14], associated fluctuations were not included. Later, the Langevin equation, that had been extensively used to study fluctuations in dissipative dynamics [15], has been

adopted to study the dynamical diffusion over the conditional saddle to estimate the formation probability, i.e. the probability to reach the compound configuration from the contact point [16, 17, 18, 19, 20]. This leads to a more realistic energy dependence of the fusion cross-section and a better estimate of the extremely low cross-sections.

Note that the so-called Dinuclear System (DNS) model was developed in parallel [21, 22, 23]. There are also attempts to bridge it with the approach mentioned above [24, 25].

In this communication, we introduce an additional mechanism that contributes to the fusion hindrance. All models mentioned above are based on the dynamics of few collective degrees of freedom that were intuitively chosen, some diffusing over a potential barrier. This is particularly true for attempts which propose an analytical formula [16, 18, 19, 20]. However, the reduction to few variables must be grounded on theory. One way consists in the elimination of fast variables in a multidimensional system because we are generally not interested in the short time motion but rather in the fate of the system. The model is then based on a reduced number of slow variables. Several seminal articles and textbooks address the subject; see e.g. [26].

However, elimination of the fast variables induces a slip of the initial condition of the slow variables [27, 28, 29, 30, 31, 32], thus affecting the formation probability. The goal of this work is to study such an effect on the fusion hindrance in reactions leading to the synthesis of heavy and superheavy nuclei.

2. Initial slip due to the elimination of fast variables and fusion hindrance

At contact, the dinuclear system is far from equilibrium, but nucleonic degrees of freedom are assumed to be already thermalised. Thermal fluctuations are a key driver to allow some of the dinuclear system to form a compound nucleus rather than reseparate into two fragments. The former channel is generally called formation and the latter quasi-fission. The description of the shape transition from a configuration close to contact of two nuclei to the spherical compound state requires many variables that evolve dynamically. Some are known to evolve faster than others. This is particularly the case for the neck between the two nuclei close to contact as a small neck requires a large amount of

surface energy [33, 34, 35, 36, 37]. This is also the case for momenta that are quickly dissipated by the strong dissipation.

In the following, we separate the collective variables into fast and slow, in order to reduce the description to a small number of slow variables. Moreover, we shall assume that all fast variables converge to finite values. There are two possible formalisms to study the classical evolution of the system including dissipation and fluctuation: the Fokker-Planck formulation used in Ref. [31] or Langevin type equations that are equivalent. We used both of them, but in this communication we choose the latter that is generally employed to describe the formation process [16, 18].

2.1. Formalism

We assume that the model is described by the following differential equation [38]:

$$\frac{d}{dt} \begin{bmatrix} F \\ S \end{bmatrix} = \begin{bmatrix} D_f & C_{fs} \\ C_{sf} & D_s \end{bmatrix} \begin{bmatrix} F \\ S \end{bmatrix} + \begin{bmatrix} R_f(t) \\ R_s(t) \end{bmatrix}, \quad (1)$$

where F is an n_f -dimension vector with the fast variables and S an n_s -dimension vector with the slow ones. R_f and R_s are respectively n_f - and n_s -dimension vectors with the random forces. D_f is an $n_f \times n_f$ drift matrix, D_s an $n_s \times n_s$ one, C_{fs} and C_{sf} are respectively $n_f \times n_s$ and $n_s \times n_f$ coupling matrices.

For the sake of simplicity, we have assumed that the model is linear and put the asymptotic values of the fast variables to zero. The random forces auto-correlation functions are defined by a matrix that could be determined with the dissipation-fluctuation theorem

$$\left\langle \begin{bmatrix} R_f(t) \\ R_s(t) \end{bmatrix} \cdot \begin{bmatrix} R_f(t'), R_s(t') \end{bmatrix} \right\rangle = \begin{bmatrix} \rho_f & \rho_{fs} \\ \rho_{sf} & \rho_s \end{bmatrix} \delta(t-t'). \quad (2)$$

The differential equations for the fast variables can be formally integrated into

$$F(t) = e^{D_f t} \cdot F_0 + \int_0^t e^{D_f(t-t')} \cdot C_{fs} \cdot S(t') dt' + \int_0^t e^{D_f(t-t')} \cdot R_f(t') dt', \quad (3)$$

where F_0 is a vector with the initial values of the fast variables. Thus, the set of differential equations satisfied by the slow variables reads

$$\dot{S} = D_s S + C_{sf} \int_0^t e^{D_f(t-t')} \cdot C_{fs} \cdot S(t') dt' + C_{sf} e^{D_f t} \cdot F_0 + C_{sf} \int_0^t e^{D_f(t-t')} \cdot R_f(t') dt' + R_s(t), \quad (4)$$

which corresponds to a Generalised Langevin equation with a memory kernel. Here, the first two terms of

the r.h.s. govern the drift of the slow variables and the last two ones their diffusion by the random forces. The third term is responsible for the initial slip, as we shall see.

Considering the difference of time scale between the two sets of variables, the integral in the second term of the r.h.s. of Eq. (4) can be approximated by

$$\int_0^t e^{D_f(t-t')} \cdot C_{fs} \cdot S(t') dt' \simeq -D_f^{-1} \cdot C_{fs} \cdot S(t), \quad (5)$$

thanks to the Laplace approximation. This leads to a Markovian set of differential equations for the slow variables,

$$\dot{S} \simeq \left[D_s - C_{sf} \cdot D_f^{-1} \cdot C_{fs} \right] \cdot S + C_{sf} \cdot e^{D_f t} \cdot F_0 - C_{sf} \cdot D_f^{-1} \cdot R_f(t) + R_s(t). \quad (6)$$

We shall now introduce an intermediate time τ , long for the fast variables and short for the slow ones. At time τ fast variables have converged to their asymptotic limit. Integration of Eq. (6) over the time τ leads to

$$S(\tau) \simeq S_0 - C_{sf} \cdot D_f^{-1} \cdot F_0, \quad (7)$$

at the zeroth order in τ . Here, S_0 is a vector with the initial values of the slow variables. Thus, once the fast variables have converged, the slow variables start to move at their own pace, but with slipped initial conditions due to their coupling to the fast variables. Their evolution after time τ is governed by a Markovian Langevin equation,

$$\dot{S} = \left[D_s - C_{sf} \cdot D_f^{-1} \cdot C_{fs} \right] \cdot S + R'_s(t), \quad (8)$$

which is the same as Eq. (6) without the term that has vanished at time τ and with

$$\langle R'_s(t) \cdot R'^T_s(t') \rangle = \left(\rho_s + C_{sf} \cdot D_f^{-1} \cdot \rho_f \cdot D_f^{-1T} \cdot C_{sf}^T - C_{sf} \cdot D_f^{-1} \cdot \rho_{fs} - \rho_{sf} \cdot D_f^{-1T} \cdot C_{sf}^T \right) \delta(t-t'). \quad (9)$$

Here, the subscript T means transposed. The dynamical equation has no memory kernel anymore, but the initial condition includes effects of the past elimination of the fast variables.

When the slow variables are close to a stable equilibrium, they end up at equilibrium, whatever the initial condition and the relaxation time is not affected because it is longer than τ . Thus, the slip of the initial conditions can be safely neglected. However, this is not the case for chaotic systems or near a bifurcation. The impact of this initial slip on various problems has been studied in Refs. [27, 28, 29, 32]. Here, we shall study the specific case of slow variables facing a potential barrier. A small change in their initial position has an impact on the size of the barrier that has to be overcome. It thus affects the crossing probability.

2.2. Application to fusion hindrance

The formation step of the fusion process is generally studied with the Langevin formalism. However, various models ranging from multidimensional formalism [16, 17, 39, 40] to a simple over-damped equation [19, 20] are used. The latter is assumed to be an intuitive simplification of the former. Here, we shall consider the reduction to a one-dimension over-damped model.

2.2.1. A simple model Let us consider the case of the formation of a compound system from a symmetric reaction in order to retain only two variables, ε , the neck variable and s , the separation between the two nuclei. We also assume that the potential map consists of two parabolas, a well for the neck characterised by the angular frequency ω_ε and a barrier for the separation, with the angular frequency ω_s , as in Ref. [35]. Assuming that these two variables are only coupled through the friction tensor β , the coupled Langevin equations read

$$\ddot{\varepsilon} + \beta_{\varepsilon\varepsilon}\dot{\varepsilon} + \beta_{\varepsilon s}\dot{s} + \omega_\varepsilon^2\varepsilon = r_\varepsilon(t) \quad (10)$$

$$\ddot{s} + \beta_{ss}\dot{s} + \beta_{s\varepsilon}\dot{\varepsilon} - \omega_s^2s = r_s(t). \quad (11)$$

Here $r_\varepsilon(t)$ and $r_s(t)$ are the Markovian random forces.

It was shown in Refs. [33, 34, 35, 36, 37] that the neck between the two nuclei close to contact quickly disappears compared to the evolution of the separation. Moreover, when the friction tensor is strong enough, the momenta quickly thermalise and the Langevin equation is sometimes replaced by its over-damped version. These are also two assumptions of the ‘‘fusion by diffusion’’ model that we shall revisit later. Thus, assuming that the coefficients entering the previous equations are such that ε , $\dot{\varepsilon}$ and \dot{s} can be considered as fast variables and s as a slow one, the previous set of equations can be rewritten as

$$\frac{d}{dt} \begin{bmatrix} \dot{\varepsilon} \\ \varepsilon \\ \dot{s} \\ s \end{bmatrix} = \begin{bmatrix} -\beta_{\varepsilon\varepsilon} & -\omega_\varepsilon^2 & -\beta_{\varepsilon s} & 0 \\ 1 & 0 & 0 & 0 \\ -\beta_{s\varepsilon} & 0 & -\beta_{ss} & +\omega_s^2 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \dot{\varepsilon} \\ \varepsilon \\ \dot{s} \\ s \end{bmatrix} + \begin{bmatrix} r_\varepsilon(t) \\ 0 \\ r_s(t) \\ 0 \end{bmatrix}. \quad (12)$$

Then, application of the above procedure reduces the dynamics to a single over-damped Langevin equation

$$\dot{s} = \frac{\omega_s^2}{\beta_{ss}}s + \frac{1}{\beta_{ss}}r_s(t), \quad (13)$$

with a slipped initial condition

$$s(\tau) = s_0 + \frac{\dot{s}_0}{\beta_{ss}} + \frac{\beta_{s\varepsilon}}{\beta_{ss}}\varepsilon_0. \quad (14)$$

We obtained the same result using the Fokker-Planck equation and the Nakajima-Zwanzig projection method [41].

The first term of the r.h.s. of Eq. (14) is the initial separation s_0 , the second term corresponds to the elimination of the initial velocity \dot{s}_0 and the third term to the elimination of the neck from its initial value ε_0 . The last two terms represent the initial slip. Thus, the slip due the neck just adds up to the slip due to the initial velocity, as equations are linear.

Eventually, the mean trajectory satisfying Eq. (13), which is equivalent to a Smoluchowski equation, reads

$$\langle s(t) \rangle = \left(s_0 + \frac{\dot{s}_0}{\beta_{ss}} + \frac{\beta_{s\varepsilon}}{\beta_{ss}}\varepsilon_0 \right) e^{\frac{\omega_s^2}{\beta_{ss}}t}, \quad (15)$$

with a slipped initial condition that is necessary to mimic the solution of the full Langevin equation. The random force induces fluctuations around this mean trajectory that are characterised by the variance

$$\sigma_s^2(t) = \frac{T}{m_s\omega_s^2} \left(e^{2\frac{\omega_s^2}{\beta_{ss}}t} - 1 \right). \quad (16)$$

Here, T is the temperature with the Boltzmann constant set to 1 and m_s is the inertia term for the separation variable.

Consequently, the elimination of the neck variable tends to drive the initial condition away from the saddle located in $s = 0$ as $\varepsilon_0 > 0$, thus increasing the hindrance phenomenon. However, the initial velocity $\dot{s}_0 < 0$ tends to bring the initial position closer to the top of the barrier, thus decreasing the hindrance phenomenon. The latter effect depends on the remaining kinetic energy at the entrance of the formation phase.

As the elimination of the neck was treated in Ref. [35], we shall focus on the other contribution.

2.2.2. Energy dependence of the initial slip The contribution to the initial slip that depends on the initial velocity or kinetic energy corresponds to the elimination of the fast momentum when the friction is large enough. Thus, it connects the full Langevin equation used in Refs. [16, 18] to its approximated over-damped version for strong friction used in Refs. [19, 20]. The former is equivalent to the Klein-Kramers equation and the latter to the Smoluchowski equation. Connection between these two equations has already been studied in the literature; see e.g. [30, 42, 43, 44]. Here, we focus on the initial slip and its impact on the formation probability for the separation variable s without coupling to the neck ($\beta_{s\varepsilon} = \beta_{\varepsilon s} = 0$).

Knowing the mean trajectory and the variance, the probability to cross the potential barrier reads [16, 18]

$$P(t) = \frac{1}{2} \operatorname{erfc} \left[-\frac{\langle s(t) \rangle}{\sqrt{2}\sigma_s(t)} \right]. \quad (17)$$

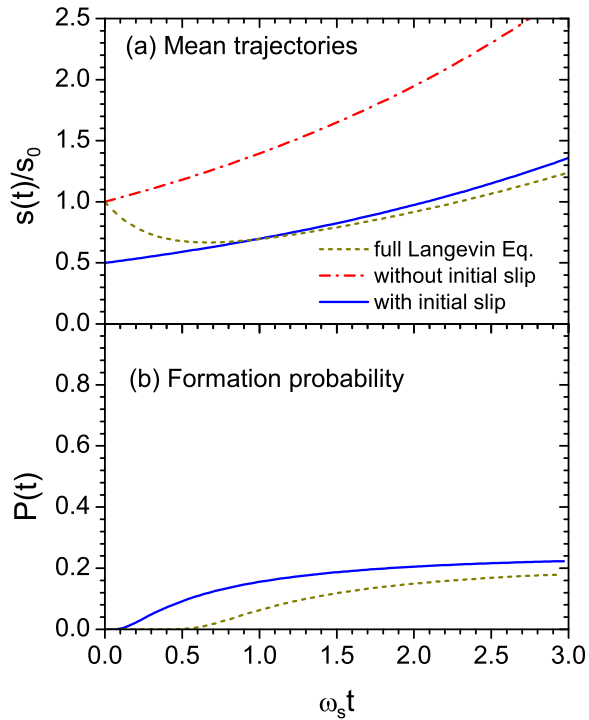


Figure 1. Top: Mean trajectory as a function of time calculated with the full Langevin equation (brown dashed line), the overdamped equation without initial slip (red dashed dotted line) and with initial slip (blue solid line).

Bottom: Formation probability as a function of time.

Here $\beta_{ss}/\omega_s = 3$, $\dot{s}_0/\omega_s s_0 = -1.5$ and $T/B = 0.5$, with B the barrier height.

The mean trajectory and the variance could be either the approximated solutions given in Eqs. (15-16) or the exact solutions of the Langevin equation [18]. Figure 1 exhibits the approximate mean trajectory with and without the initial slip \dot{s}_0/β_{ss} . It appears that without the slipped initial condition, the long-time behaviour of the approximate and exact trajectories diverge. With the slipped initial condition, the two solutions differ at short time, but have the same asymptotic trend. The same remark applies to the formation probability. Note that the smaller ω_s/β_{ss} the better the asymptotic agreement, since fast and slow time scales are well separated.

In Fig. 1, the initial velocity is supposed to be small and the mean trajectory does not cross the barrier located at $s = 0$. If this initial velocity increases to values that allow the mean trajectory to overcome the barrier, the slipped initial condition is on the other side of the barrier, as can be seen in Fig. 2. Consequently, the formation probability of the approximate solution with the initial slip starts from 1 which is not realistic. However, the asymptotic behaviour is correct.

Note that for both figures, the formation

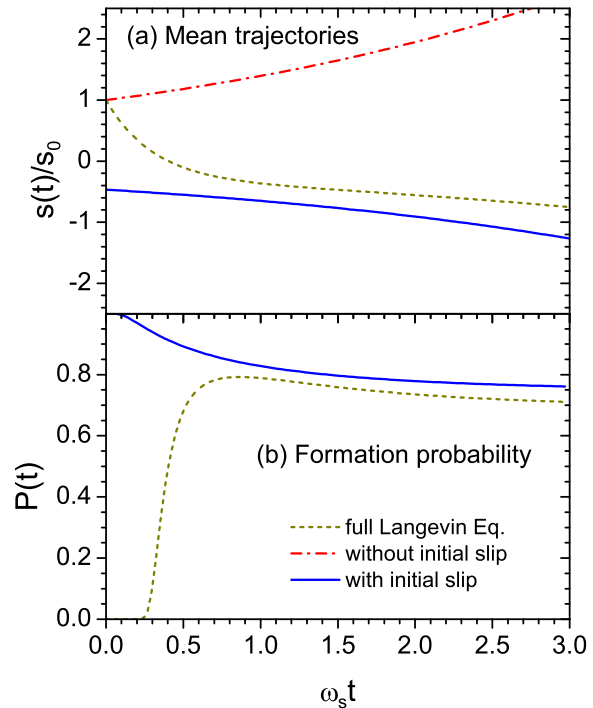


Figure 2. Same as Fig. 1, but with a large initial velocity, $\dot{s}_0/\omega_s s_0 = -4.4$.

probability without an initial slip is too small to appear. These examples show that the slip of the initial condition has a great influence on the formation probability and the cross-section, thus it should be taken into account for a correct description of the fusion process when an over-damped equation is used.

3. Fusion by diffusion model revisited

In the “fusion by diffusion” model [19, 20], a one dimension Smoluchowski equation is used to describe the formation step and a phenomenological initial shift is introduced and adjusted in order to reproduce experimental data. A systematics over several reactions [45, 46, 47, 48, 49] exhibits a somehow regular behaviour, for both cold and hot fusion reactions. The initial separation between the nuclei at contact diminishes when the centre of mass energy increases. Such a trend is similar to what we found in the previous section.

To link our results with the empirical shift used in the “fusion by diffusion” model one needs to determine \dot{s}_0 or the remaining kinetic energy at contact, just after the capture phase.

3.1. Remaining kinetic energy after capture

In the “fusion by diffusion” model [19, 20, 45, 46, 47, 48, 49], the capture cross section is determined by

$$\sigma_{cap} = \int_0^{\infty} \sigma_c(B_C) f(B_C) dB_C, \quad (18)$$

which consists in folding the classical formula

$$\sigma_c = \pi R_c^2 \left(1 - \frac{B_C}{E_{cm}}\right) \theta(E_{cm} - B_C), \quad (19)$$

by the following Coulomb barrier distribution

$$f(B_C) = \frac{1}{\sqrt{2\pi}\sigma_B} \exp\left[-\frac{(B_C - \bar{B}_C)^2}{2\sigma_B^2}\right]. \quad (20)$$

Here, $\theta(E_{cm} - B_C)$ is the Heavyside step function. The parameters R_c , \bar{B}_C and σ_B depend on other parameters that are adjusted to experimental data [20, 50].

Within the same model, we can also calculate the mean remaining kinetic energy of the captured events defined as the centre of mass kinetic energy minus the Coulomb barrier and the rotational energy. Summing over all impact parameters and Coulomb barriers, we get

$$\langle K_r \rangle = \sqrt{\frac{2}{\pi}} \sigma_B \frac{\frac{\sqrt{\pi}}{4} (2X^2 + 1)(1 + \text{erf}(X)) + \frac{X}{2} \exp(-X^2)}{X(1 + \text{erf}(X)) + \frac{1}{\sqrt{\pi}} \exp(-X^2)}, \quad (21)$$

with

$$X = \frac{E_{cm} - \bar{B}_C}{\sqrt{2}\sigma_B}. \quad (22)$$

When $E_{cm} \gg \bar{B}_C$, $\langle K_r \rangle \simeq \frac{1}{2}(E_{cm} - \bar{B}_C)$.

Figure 3 shows the remaining kinetic energy at the top of the Coulomb barrier as a function of X defined above. It appears that when $E_{cm} > \bar{B}_C$, the asymptotic behavior is quickly reached. When $E_{cm} < \bar{B}_C$, only events with a Coulomb barrier below E_{cm} contribute and the remaining kinetic energy is small.

3.2. Initial conditions of the formation step

In the “fusion by diffusion” model [45, 46, 47, 48, 49], the injection point of the formation phase which corresponds to the shifted separation has been considered having a linear behavior with $E_{cm} - \bar{B}_C$. However, according to the present analysis, it should rather be defined as

$$s_{inj} = s_0 - \frac{c}{\beta_{ss}} \sqrt{\frac{2\langle K_r \rangle}{\mu c^2}}, \quad (23)$$

where μ is the reduced mass of the system and c the light-speed.

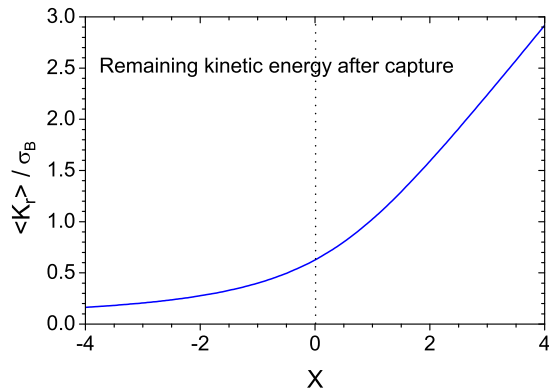


Figure 3. Remaining mean kinetic energy in σ_B unit at the top of the Coulomb barrier as a function X which depends on the centre-of-mass energy, see Eq. (22).

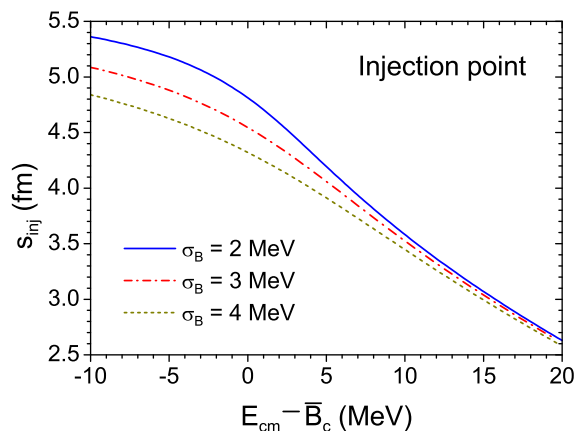


Figure 4. Evolution of the injection point s_{inj} calculated with Eq. (23) as a function of the centre of mass energy in MeV. Here, we arbitrarily set $s_0 = 6$ fm, $\beta = 2 \times 10^{21}$ s $^{-1}$ and $\mu = 40$ u. The three curves are for $\sigma_B = 2$ MeV (blue solid line), $\sigma_B = 3$ (red dot dashed line) MeV and $\sigma_B = 4$ MeV (brown dashed line).

Figure 4 shows the initial separation of the two nuclei given in Eq. (23), as a function of the centre of mass energy for a given reaction. The part of the graph with $E_{cm} < \bar{B}_C$ mostly corresponds to the cold fusion domain [45, 48] and the part with $E_{cm} > \bar{B}_C$ mostly corresponds to the hot fusion one [47], even though the two domains overlap around $E_{cm} \simeq \bar{B}_C$. The slopes differ significantly in the two energy domains, as for the phenomenological shift extracted in Refs [45, 46, 47, 48]. Figure 4 also exhibits the influence of the standard deviation of the Coulomb barriers distribution σ_B that differs from system to system. This parameter has a greater impact for the cold fusion domain than for the hot fusion one. This would explain the larger scattering of the points observed phenomenologically for cold fusion reactions.

The phenomenological shift extracted in Refs [45, 46, 47, 48] is an umbrella parameter that accounts

for all the shortcomings of the model. In particular, it depends on the fission barriers chosen to calculate the survival probabilities as it can be seen when comparing the results of Refs. [48] and [45]. In Ref. [49], the difference of slopes between cold and hot fusion is partially explained by the strong deformation of the actinide target nuclei used for hot fusion reactions. Thus, the present work only provides a partial explanation.

This remaining kinetic energy is responsible for the displacement of the initial condition in the over-damped description. At time τ it is completely damped when the slow variable, i.e. the separation distance here, starts to evolve without any initial inertia from the slipped position. Thus, the remaining kinetic energy has been changed into excitation energy by the strong dissipation and should be taken into account in the temperature.

4. Conclusions and discussions

Elimination of the fast variables gives rise to an initial slip to the coupled slow variables that is generally neglected or even ignored. When the slow variables are initially departed from their equilibrium position, as it is most frequently the case in physics, this is not a problem. However, when the slow variables face a bifurcation, a potential barrier or for chaotic systems, a small change in the initial conditions can have a significant impact on the long time behaviour of the system. In such conditions, the initial slip should be taken into account.

In this communication, we found that this slip of the initial conditions significantly contributes to the fusion hindrance observed in heavy-ion collisions. This contribution can partially explain the initial shift introduced phenomenologically in the formation phase of the “fusion by diffusion” model [19, 20, 45, 46, 47, 48, 49]. The impact is expected to be important as a shift of 1 fm of the initial condition of the formation probability leads to a change of about one order of magnitude of the fusion-evaporation cross-sections.

The description of the shape evolution of the dinuclear system to the compound mono-nucleus requires many variables. Whatever the description, there might be forgotten variables that are supposed to have disappeared. What are their contributions to the initial slip? We are currently working on this issue that will be addressed in another article. However, we can already mention that the faster the eliminated variable the smaller the slip. Thus, elimination of numerous very fast variables should not affect much the slow variables.

Eventually, the formula given for the initial slip is based on the elimination of fast variables that supposes

a clear separation between the characteristic times of the fast and slow variables. However, in heavy-ion reactions, fast variables are not that fast compared to the slow ones. For such cases, the approximation done in this article might be too crude. We are currently working on this problem.

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