

# Microscopic Investigation of Fusion and Quasifission Dynamics

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**Abstract.** We introduce the application of time-dependent Hartree-Fock (TDHF) theory to two key aspects of heavy-ion reaction dynamics for producing superheavy elements: fusion and quasi-fission (QF). For fusion reactions  $^{48}\text{Ca}+^{238}\text{U}$ , the capture cross sections, fusion probabilities, and evaporation-residue cross sections are calculated using TDHF theory combined with coupled-channel and fusion-by-diffusion models, and the results are found to be in reasonable agreement with available experimental data. For the QF process of  $^{48}\text{Ca}+^{249}\text{Bk}$ , we show the distribution of the fragments and investigate the impact of the tensor force, significantly enhancing the role of spherical shell effects.

## 1 Introduction

The investigation of superheavy elements (SHEs) constitutes a prominent and active frontier in modern nuclear physics [1–3]. Up to now, SHEs up to  $Z = 118$  have been produced. This was accomplished using two kinds of reactions: cold-fusion reactions, which employed  $^{208}\text{Pb}$  and  $^{209}\text{Bi}$  targets for elements up to  $Z = 113$  [4, 5], and hot-fusion reactions, which utilized  $^{48}\text{Ca}$  projectiles on actinide targets to produce elements from  $Z = 114$  to  $Z = 118$  [6–8]. Significant experimental efforts have been made to produce superheavy nuclei with  $Z = 119$  and  $Z = 120$  [3, 9–11], but no successful synthesis has yet been reported.

This lack of success stems chiefly from the prevalence of quasifission, a competing mechanism that overwhelmingly dominates in heavy systems and severely inhibits compound nucleus formation. This competition becomes particularly prominent for the synthesis of the SHEs, as the enormous Coulomb repulsion makes quasifission (QF) the dominant reaction channel. In contrast to fusion, which leads to the formation of a fully equilibrated compound nucleus (CN), the QF process involves a different trajectory. Although the colliding nuclei surpass the capture barrier, they do not amalgamate and subsequently re-separate into two fragments [12]. As a nonequilibrium mechanism, QF is characterized by several distinct features: interaction times are typically shorter than in fusion-fission, substantial mass exchange occurs, strong correlations between fragment mass and angle are observed, and a “memory” of the entrance channel properties is partially retained [13].

Conceptually, the fusion-evaporation reaction can be understood as a three-step process: (i) the capture of the projectile by the target, forming a dinuclear system; (ii) the formation of an equilibrated CN, and (iii) the de-excitation of the CN against the emission of light particles and fission. Most theoretical approaches provide a relatively con-

sistent description for the capture process [14–16]. However, the second and third steps, the formation and deexcitation of the CN, remains the most significant source of theoretical uncertainty. Predictions for the two stages from various models can differ by several orders of magnitude. The crucial stage, the formation of the CN, governs the evolution of the dinuclear system after capture, determining whether it proceeds to form a compact, fully equilibrated CN or re-separates into two fragments via QF. Therefore, a quantitative understanding of the fusion-QF competition, which determines the CN formation probability  $P_{\text{CN}}$ , is essential for making reliable predictions of SHE synthesis cross sections.

To achieve a quantitative understanding, various theoretical models have been developed. Macroscopic ones can be parameterized to reproduce known cross-section data, but their reliance on adjustable parameters and limited treatment of dynamics challenge their predictive power for unmeasured systems. In contrast, the microscopic TDHF approach offers insights into the underlying dynamics [17–22] and has been successfully applied to many aspects of low-energy heavy-ion collisions, including fission [23–26], fusion [27–36], QF [37–42] and multinucleon transfer reactions [43–46]. Although TDHF is not suitable for the full fusion-evaporation process or quantum tunneling phenomena such as sub-barrier fusion, its simulations can provide the main ingredients for coupled-channels calculations [18, 47] and diffusion processes [35, 48, 49].

In this contribution, we introduce the results from Ref. [48] regarding the calculation of evaporation cross sections of the hot fusion reaction  $^{48}\text{Ca} + ^{238}\text{U}$ , where the TDHF simulations are used to provide the inputs for capture and fusion processes. We combine TDHF with both the coupled-channel (CC) and fusion-by-diffusion (FbD) approaches to calculate the cross sections of the three-step in fusion reactions. In parallel, we also show the quasifission process of  $^{48}\text{Ca} + ^{249}\text{Bk}$  from Ref. [40] via TDHF

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calculations, incorporating the orientation effects of deformed reactants. By analyzing the resulting fragment yield distributions with different Skyrme forces, we aim to extract the specific influence of the tensor force on the QF fragments.

## 2 Theoretical Framework

In the TDHF theory, the dynamic process is described by the evolution of the one-body density  $\hat{\rho}$ , which is obtained by solving the TDHF equation

$$i\hbar \frac{\partial}{\partial t} \hat{\rho} = [\hat{H}(\hat{\rho}), \hat{\rho}], \quad (1)$$

where  $\hat{H}$  represents the single-particle Hamiltonian derived from the effective interaction. The TDHF theory describes the collective motion semiclassically, omitting the quantum tunneling of the many-body wave function. Consequently, when calculating capture cross sections, a common and effective approach is to use internuclear potentials derived from microscopic calculations such as frozen density approximation [31], density constrained TDHF (DC-TDHF) [22, 35, 50], or density constrained frozen HF (DC-FHF) [36, 48, 51], as the input of the coupled-channels code CCFULL [52] to calculate the penetration probability.

For hot-fusion reactions, the actinide target nuclei are often strongly deformed; therefore, the orientation effects must be explicitly considered. In Ref. [48] we utilize the DC-FHF method to calculate the internuclear potential directly as a function of the target's orientation. In the DC-FHF method, the HF calculations are performed with the constraint that the total proton  $p$  and neutron  $n$  densities are the same as those of the ground state of the projectile and target

$$\delta \left( H - \int d^3r \sum_{q=p,n} \lambda_q(\mathbf{r}) [\rho_q^p(\mathbf{r}; \theta_P) + \rho_q^T(\mathbf{r} - \mathbf{R}; \theta_T)] \right), \quad (2)$$

= 0

where  $\rho^p$  and  $\rho^T$  are the densities of the projectile and target for a given orientation. These densities are achieved by performing Eulerian rotations of Slater determinants in a three-dimensional Cartesian system [53].  $\theta_P$  ( $\theta_T$ ) denotes the angle between the symmetry axis of the deformed projectile (target) and the collision axis.  $\mathbf{R}$  is the vector between the centers of mass of the projectile and target. This variation procedure results in a unique Slater determinant  $\Phi(\mathbf{R})$ . The internuclear potential is then given by:

$$V(\mathbf{R}; \theta_P, \theta_T) = \langle \Phi(\mathbf{R}) | H | \Phi(\mathbf{R}) \rangle(\theta_P, \theta_T) - E_P - E_T, \quad (3)$$

where  $E_P$  and  $E_T$  are the ground state binding energies of the projectile and target, respectively.

The penetration probabilities  $T_J(E_{c.m.}, \theta_T, \theta_P)$  for each partial wave  $J$  are obtained by solving the Schrödinger equation using the incoming wave boundary condition method [52]. The orientation-average cross-section is

given as

$$\sigma_{\text{cap}}(E_{c.m.}) = \int_0^1 d \cos(\theta_P) \int_0^1 d \cos(\theta_T) \times \frac{\pi}{k^2} \sum_J (2J+1) T_J(E_{c.m.}, \theta_T, \theta_P), \quad (4)$$

where  $k = \sqrt{2\mu E_{c.m.}}/\hbar$  is the wave number.

The fusion probability  $P_{\text{CN}}(\theta_P, \theta_T, E_{c.m.}, J)$  is calculated using the FbD model. The key input for this model, the injection point, is estimated from TDHF simulations. The fusion cross section  $\sigma_{\text{fus}}$  is then given by

$$\sigma_{\text{fus}}(E_{c.m.}) = \int_0^1 d \cos(\theta_P) \int_0^1 d \cos(\theta_T) \times \frac{\pi}{k^2} \sum_J (2J+1) T_J(E_{c.m.}, \theta_T, \theta_P) \times P_{\text{CN}}(\theta_P, \theta_T, E_{c.m.}, J). \quad (5)$$

To facilitate comparison with experimental data, the effective fusion probability  $P_{\text{fus}}$  is defined as the ratio

$$P_{\text{fus}}(E_{c.m.}) = \frac{\sigma_{\text{fus}}(E_{c.m.})}{\sigma_{\text{cap}}(E_{c.m.})}. \quad (6)$$

The survival probability  $W_{\text{sur}}(E_{\text{CN}}^*, x, J)$  of the CN is calculated using a statistical model [48, 54, 55] that considers the competition between  $x$ -neutron emission and fission. The final evaporation residue (ER) cross section  $\sigma_{\text{ER}}$  for the  $xn$  channel is

$$\sigma_{\text{ER}}(E_{c.m.}, x) = \int_0^1 d \cos(\theta_P) \int_0^1 d \cos(\theta_T) \times \frac{\pi}{k^2} \sum_J (2J+1) T_J(E_{c.m.}, \theta_T, \theta_P) \times P_{\text{CN}}(\theta_P, \theta_T, E_{c.m.}, J) W_{\text{sur}}(E_{\text{CN}}^*, x, J). \quad (7)$$

For the QF cross section or yield for a specific reaction channel, different impact parameters and orientations result in distinct yield contributions. These contributions are quantified using

$$\sigma_{\lambda} \propto \int_{b_{\text{min}}}^{b_{\text{max}}} b db \int_0^{\pi/2} d\beta \sin(\theta_T) P_b^{(\lambda)}(\theta_T), \quad (8)$$

where  $\lambda$  denotes a specific reaction channel, and  $P_b^{(\lambda)}(\theta_T)$  is the probability corresponding to a given impact parameter  $b$  and orientation angle  $\theta_T$ . This probability is either 0 or 1 for the reaction channel  $\lambda$  [20, 40, 42].

## 3 Results and Discussions

We first investigate the capture dynamics of the  $^{48}\text{Ca} + ^{238}\text{U}$  system, in which the  $^{238}\text{U}$  target is prolate-deformed. Using the DC-FHF method, we obtain the internuclear potentials for seven orientations of  $^{238}\text{U}$  in the range  $[0, \pi/2]$ . The capture cross section was then computed from these potentials using the orientation-averaged formalism. As illustrated in Fig. 1(a), the orientation-averaged capture cross sections  $\sigma_{\text{cap}}$  (solid red line) provide a reasonable

description of the experimental data (solid circles) [56], with good agreement at energies above 200 MeV. For incident energies smaller than 190 MeV, our results are also better than those of the empirical coupled-channels (ECC) model [57]. The plot also clearly highlights the strong dependence on the orientation of the deformed  $^{238}\text{U}$  target. The cross section for a near-tip collision ( $\theta = 6.2^\circ$ , dashed line) is substantially enhanced compared to that of a near-side collision ( $\theta = 80.5^\circ$ , dotted line). This enhancement is a direct consequence of the significantly lower capture barrier associated with the tip orientation.

Having established the capture cross section  $\sigma_{\text{cap}}$ , we next compute the orientation-averaged fusion cross section  $\sigma_{\text{fus}}$  (black line in Fig. 1(b)). This calculation was performed using the FbD model [15]. A key methodological strength is that the sole input parameter required by the FbD model—the injection distance—was directly extracted from our microscopic TDHF simulations. From this computed  $\sigma_{\text{fus}}$  and the previously calculated  $\sigma_{\text{cap}}$ , we then derived the effective fusion probability,  $P_{\text{fus}} = \sigma_{\text{fus}}/\sigma_{\text{cap}}$ , which is plotted as the red line. The resulting  $P_{\text{fus}}$  values are found to be in the range of  $(2 - 6) \times 10^{-4}$ . Concurrently, the calculated  $\sigma_{\text{fus}}$  increases slowly with incident energy.

In the third and final stage of our calculation, we determine the evaporation-residue cross sections, shown in Fig. 1(c) for the  $3n$  (black line) and  $4n$  (red line) channels. These cross sections are obtained by combining the calculated fusion cross section  $\sigma_{\text{fus}}$  with the survival probability  $W_{\text{sur}}$ , which is evaluated within a statistical model describing the competition between fission and neutron emission during the de-excitation of the compound nucleus. The required fission barriers and neutron-separation energies are taken from the microscopic-macroscopic calculations of Ref. [58]. The calculated results provide a reasonable description of the available experimental data for both channels. The better agreement for the  $3n$  channel near  $E_{\text{c.m.}} \approx 195$  MeV may be related to the stronger sensitivity of the  $4n$  survival probability to the excitation energy. The adopted fission barrier height is higher for  $^{283}\text{Cn}$  (about 4.6 MeV) than for  $^{282}\text{Cn}$  (about 3.7 MeV), which favors survival in the  $3n$  channel. We also note that the reported  $4n$  value at  $E_{\text{c.m.}} \approx 195$  MeV is an upper limit, and our calculated result remains below it. Overall, these results support the hybrid framework employed here as an effective approach for describing the hot-fusion reaction process.

In the study of QF dynamics, the fragment mass-angle distributions (MADs) are crucial experimental observables. These distributions provide profound insights into the reaction mechanism, particularly by revealing the role of quantum shell effects in shaping the characteristics of the fragments [59]. To theoretically derive the MADs and the corresponding fragment yield distributions via TDHF simulations, extensive TDHF calculations are imperative [20, 40, 42]. For the  $^{48}\text{Ca} + ^{249}\text{Bk}$  system, as reported in Ref. [40], we systematically sampled five distinct initial orientations of the deformed  $^{249}\text{Bk}$  target. For each orientation, the TDHF calculations are performed by considering a wide range of impact parameters  $b$ , which

begins from central collisions ( $b = 0$ ) up to grazing trajectories where elastic scattering occurs. Figure 2 provides a direct comparison between calculations with the Skyrme interactions SLy5t [60], which includes the tensor force, and the SLy5 set [61]. The incident energy is  $E_{\text{c.m.}} = 234$  MeV in the center-of-mass frame. A clear enhancement of the neutron shell effects due to the tensor force is immediately apparent. The mass-angle correlation plot [Fig. 2(a)] reveals a pronounced clustering of QF fragments from the SLy5t simulation along the  $N = 126$  magic shell closure. This feature is much less distinct in the SLy5 calculation. This observation is quantified in the fragment yield distribution [Fig. 2(c)], where the SLy5t simulation exhibits a sharp peak centered precisely at  $N = 126$ . In contrast, the SLy5 calculation peaks at a lower value of  $N \approx 122$ , indicating that the  $N = 126$  shell closure plays a less dominant role in the dynamics without the tensor force.

A parallel and equally significant effect is also observed for the proton. The SLy5t fragments [Fig. 2(b), blue points] are systematically concentrated closer to the  $Z = 82$  magic number than their SLy5 counterparts. This is corroborated by the proton yield distribution in Fig. 2(d). The SLy5t yield peaks are near  $Z = 82$ , whereas the SLy5 calculation is centered at a lower  $Z \approx 79$ . Collectively, these results provide strong evidence that the inclusion of the tensor force significantly amplifies the influence of the  $N = 126$  and  $Z = 82$  quantum shell closures, strongly driving the QF dynamics toward the production of fragments in the vicinity of the doubly-magic  $^{208}\text{Pb}$ .

## 4 Summary

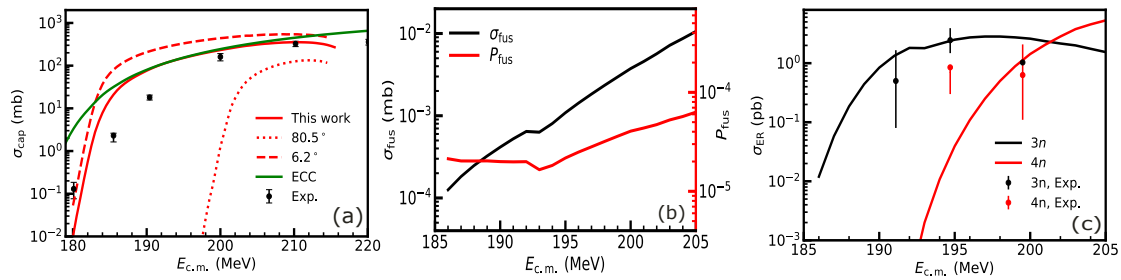
We have employed the microscopic TDHF theory, in conjunction with the coupled-channel and FbD models, to investigate the capture and fusion processes in the hot-fusion reaction  $^{48}\text{Ca} + ^{238}\text{U}$ . For this reaction, our calculated capture cross sections are in good agreement with the experimental data. Furthermore, by accounting for the survival probability of the compound nucleus using a statistical model, our calculations successfully reproduce the experimental evaporation-residue cross sections. We also explored the QF dynamics in the  $^{48}\text{Ca} + ^{249}\text{Bk}$  reaction using TDHF simulations with and without the tensor force. It is revealed that the tensor force enhances the spherical shell effects. This enhancement is clearly manifested with more fragments produced near the magic  $N = 126$  neutron shell and approaching  $Z = 82$  proton shell.

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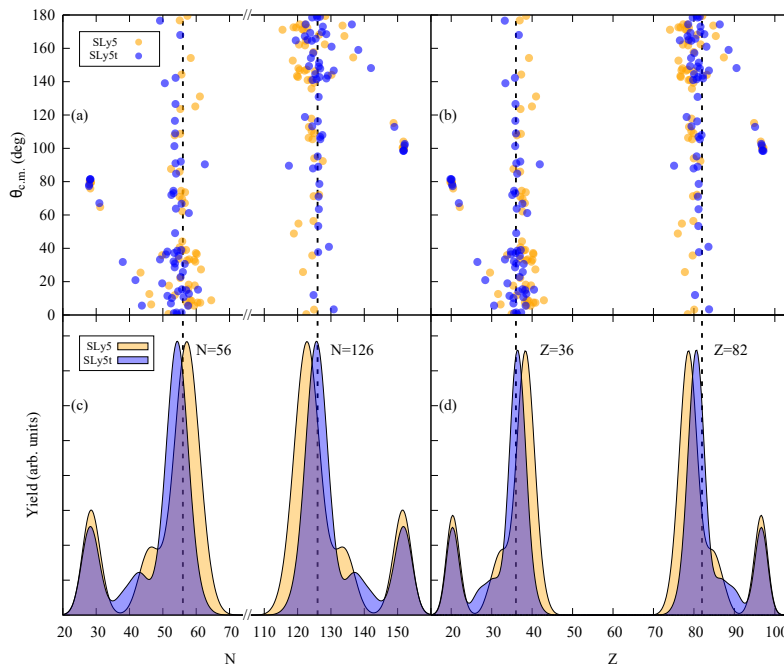
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**Figure 1.** Theoretical results for the  $^{48}\text{Ca} + ^{238}\text{U}$  reaction as a function of the center-of-mass incident energy  $E_{c.m.}$ . (a) Capture cross sections  $\sigma_{\text{cap}}$ . The orientation-averaged results (red solid line), tip ( $\theta = 9.5^\circ$ ) and side ( $\theta = 83.8^\circ$ ) orientations, the ECC model (green line), and experimental data (solid circles) are shown. (b) Orientation-averaged fusion cross sections  $\sigma_{\text{fus}}$  (black line) and effective fusion probabilities  $P_{\text{fus}}$  (red line). (c) Evaporation-residue cross sections  $\sigma_{\text{ER}}$  for the  $3n$  (black line) and  $4n$  (red line) channels, compared with experimental data (points). Taken from Ref. [48].



**Figure 2.** Quasifission reaction for the  $^{48}\text{Ca} + ^{249}\text{Bk}$  at  $E_{c.m.} = 234$  MeV. (a) Scattering angle  $\theta_{c.m.}$  versus fragment neutron number ( $N$ ). (b)  $\theta_{c.m.}$  versus fragment proton number ( $Z$ ). (c) Fragment neutron number yield. (d) Fragment proton number yield. In all panels, calculations including the tensor force (SLy5t, blue points/shade) are compared with those omitting it (SLy5, orange points/shade). Vertical dashed lines mark the positions of key shell closures at  $N = 56, 126$  and  $Z = 36, 82$ . Taken from Ref. [40].

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