Quantum calculations of Coulomb reorientation for sub-barrier fusion

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Classical mechanics and Time Dependent Hartree-Fock (TDHF) calculations of heavy ions collisions are performed to study the rotation of a deformed nucleus in the Coulomb field of a collision partner. We show that this Coulomb reorientation is *independent* on the charges and the relative energy of the partners. It only depends upon the deformations and the respective masses. Furthermore this reorientation modifies strongly the fusion cross-section around the barrier for light deformed nuclei on heavy collision partners. For such nuclei a hindrance of the sub-barrier fusion is predicted.

Tunneling, the slow "quantum leak" through a classical barrier, is an intriguing phenomenon in nature. In 1928, Gamow discovered this effect looking for an explanation of the alpha radioactivity [1]. Hence, tunnelling is one of the foundations of quantum mechanics. However, the tunneling of complex systems remains to be understood. As in the Gamow times nuclear physics is providing one of the most challenging field to understand the tunneling phenomenon. In particular, fusion reaction cross sections involving massive nuclei at, or below, the Coulomb barrier are, in some cases, orders of magnitude over expectations from one dimensional quantum tunneling predictions. Couplings between the internal degrees of freedom and the relative motion deeply modifies the tunneling phenomenon [2]. Neutron transfer, excitation of low-lying vibrational and rotational states, neck formation, zero-point motion and polarization of collective surface vibration as well as static deformation have been identified as key inputs in the understanding of this sub-barrier fusion enhancement [3].

This enhancement may become essential when one is using fusion to produce very rare elements such as super-heavy nuclei. As pointed out in [4,5], for nuclei with a significant static quadrupole deformation, the main effects are i) on the barrier height (geometrical effect) since the barrier is lower in the elongated direction and ii) on the reorientation of the deformed nucleus (rotational effect) under the torque produced by the long-range Coulomb force.

In [6–12], fusion excitation functions were measured for ^{16}O (spherical) + $^{144-154}$Sm reactions around the Coulomb barrier. ^{144}Sm is spherical whereas ^{154}Sm is prolate with ($\beta_2 \approx 0.3$). The data were interpreted as arising from the different orientations of the deformed collision partner. An enhancement of the fusion probability is observed when the deformation axis of the prolate nucleus is parallel to the collision axis ("parallel collision"); and a hindrance is seen when the two axis are nearly perpendicular ("perpendicular collision"). In these studies, however, the assumption of an *isotropic orientation distribution* of the deformed nucleus at contact was made i.e. the reorientation has been neglected. In an other hand, authors of ref. [13] recently argued that the Coulomb force systematically rotates the deformed nucleus toward the stable perpendicular configuration. This contradicts the classical calculations reported in refs. [14,15] which show that the reorientation is not complete.

From the quantum mechanics point of view, the reorientation is a consequence of the Coulomb excitation of rotational states. Computational techniques have been developed in the past to solve coupled channel equations for multiple Coulomb excitation [16–20] but a good understanding of the Coulomb reorientation dynamics during the approach phase is still required.

In this work we obtain a deeper insight in the Coulomb reorientation by using both classical approximations, solving analytically and numerically the equations of motion of a rigid body, and quantum approaches describing the colliding deformed nucleus within the time dependent Hartree-Fock (TDHF) approach. Then we will use these reorientation results in a coupled channel calculation in order to discuss the induced effects on the fusion cross-section.

Assuming first a classical treatment of nuclear orientation i.e. no interference between the various orientations, the fusion cross section is given by the orientation average formula [21,22]

$$\sigma_{fus.} \approx \int_{\varphi=0}^{\frac{\pi}{2}} \sigma(\varphi) \sin\varphi \, d\varphi \qquad (1)$$

where φ is the angle between the deformation and the collision axis and $\sigma(\varphi)$ is the associated cross section.

However, the Coulomb force induces a torque which, integrated over the whole history, up to the distance of closest approach D_0, rotates the initial angle φ_∞ into φ_0. Because of reorientation $\Delta\varphi = \varphi_0 - \varphi_\infty \neq 0$, the distribution of φ_0, lostes its isotropy. In this case the $\sin\varphi$ term in Eq. 1 has to be replaced by another distribution $f(\varphi_0)$.

To estimate $\Delta\varphi$, we consider the classical motion of a deformed rigid projectile in the Coulomb field of the target nucleus. We assume that the projectile of mass A_p presents a sharp surface at a radius $R(\theta) = R_0\sqrt{\alpha^{-4}\cos^2\theta + \alpha^2\sin^2\theta}$ where $R_0 = r_0\ A_p^{\frac{1}{3}}$, $r_0 = 1.2$ fm, $\alpha = 1-\varepsilon$ and $\varepsilon = \sqrt{\frac{5}{16\pi}}\beta_2$ (the deformation parameter).

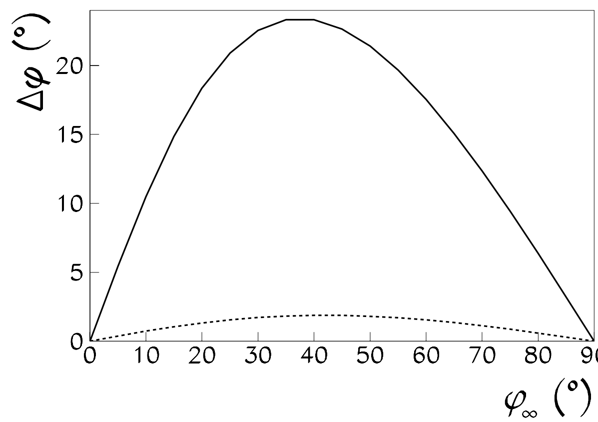

FIG. 1. Classical calculations of the total reorientation $\Delta\varphi$ (see text) of the deformed collision partner as function of its initial orientation φ_∞ for the reactions ^{24}Mg($\beta_2 = 0.4$)+^{208}Pb (solid line) and ^{154}Sm($\beta_2 = 0.3$)+^{16}O (dashed line) at the barrier. The initial distance between the centers of mass is $D_\infty = 241$ fm.

Fig. 1 shows the evolution of the reorientation as function of the initial orientation for central collisions at the barrier $B = Z_pZ_te^2/r_0\left(A_t^{1/3}+A_p^{1/3}\right)$ where Z_p (A_p) and Z_t (A_t) are the projectile and target number of protons (nucleons). The figure presents two typical asymmetric reactions of a prolate projectile on a spherical target: ^{24}Mg($\beta_2 \approx 0.4$)+^{208}Pb and ^{154}Sm($\beta_2 \approx 0.3$)+^{16}O. For symmetry reasons $\Delta\varphi = 0°$ for $\varphi = 0°$ and $90°$. The maximal reorientation $\Delta\varphi_{max}$ occurs around $45°$. For the heavy deformed projectile, ^{154}Sm, $\Delta\varphi_{max}$ is less than $2°$. In the case of ^{24}Mg, the reorientation is large, $\Delta\varphi_{max} \approx 23.3°$.

To understand this difference, an approximated expression for the maximum reorientation is derived, assuming that ε and $\Delta\varphi$ are small and thus considering $\varphi_\infty = 45°$. Computing the torque within these approximations leads to following the equation of motion for $\varphi(t)$

$$\ddot{\varphi}(t) \approx \frac{3Z_pZ_te^2\varepsilon}{mA_pD(t)^3} \tag{2}$$

where m is the nucleon mass and $D(t)$ the distance between the two nuclei. Replacing the time variable by $\xi(t) = D(t)/D_0$ and neglecting deformation and rotation on the dynamics of $D(t)$, Eq. (2) becomes

$$\frac{\partial\varphi(\xi)}{\partial\xi} + 2\xi(\xi-1)\frac{\partial^2\varphi(\xi)}{\partial\xi^2} = \frac{3\varepsilon}{\xi}\frac{A_t}{A_p+A_t}. \tag{3}$$

Only the factor $A_t/(A_p+A_t)$ remains since the initial center of mass energy E and the charges have been taken into account in $D_0 = D(0) = e^2Z_pZ_t/E$. The solution of Eq. 3 is

$$\varphi(\xi) = \varphi_\infty + 2\varepsilon\frac{A_t}{A_p+A_t}\left(\xi(2-\zeta) - 2\ln\zeta + \delta\right) \tag{4}$$

where $\zeta = 1+\sqrt{1-\frac{1}{\xi}}$ and $\delta = 2\ln 2 - 1/2$. Solved up to the distance of closest approach ($\xi = 1$), it leads to

$$\Delta\varphi = \varepsilon\frac{A_t}{A_p+A_t}\left(1+4\ln 2\right). \tag{5}$$

Eqs. (3) and (5) depend neither on projectile and target charges nor on the initial energy but only on the deformation and on the mass ratio. This counter-intuitive result, which has been exhaustively checked numerically, can be understood: the increase of the Coulomb interaction with charges (like Z_pZ_t) is compensated by an increase of the distance of closest approach, D_0. A similar balance occurs with incident energy. An increase in E simultaneously reduces D_0 and the time to interact leading to a zero net effect on the integrated reorientation. The strong difference between the two systems shown in Fig. 1 is thus only due to the difference in $A_t/\left(A_p+A_t\right)$, and not to the difference in the forces i.e. in the nuclei charges.

Fig. 2 shows the evolution of the orientation as a function of the distance between the centers of mass for the central reaction ^{24}Mg+^{208}Pb at the barrier. Results from the numerical solution of the classical dynamic of a deformed rigid body (dotted line) and approximated analytical expression Eq. 4 (dashed line) are very close. The small difference observed at the turning point can be attributed to the higher orders terms in ε not taken into account in Eq. 4. The difference at large distance is due to the fact that the numerical simulation only start at a finite value of the initial distance D_∞ ($D_\infty = 241$ fm in the presented results) while the analytical results integrate the effects from $D_\infty \to \infty$.

In order to take into account the quantal nature of the nuclei and to avoid the rigid body approximation, we have performed TDHF calculations [23–27] of the nuclear reaction. TDHF corresponds to an independent propagation of each single particle wave function in the mean field generated by the ensemble of particles. The quantal nature of the single particle dynamics is crucial at low energy both because of shell effects and of the wave dynamics. TDHF theory is optimized for the prediction of the average values of one body observables and so the deformation and the orientation should be well estimated by TDHF.

In the TDHF approach, the evolution of the one-body density matrix $\rho = \sum_{n=1}^{N}|\varphi_n\rangle\langle\varphi_n|$ is determined by a Liouville equation,

$$i\hbar\frac{\partial}{\partial t}\rho - [h(\rho), \rho] = 0 \quad (6)$$

where $h(\rho)$ is the mean-field Hamiltonian. We have used the code built by P. Bonche and coworkers [28] with an effective Skyrme mean-field [29]. Two different parametrizations were used, SkM^* [30] and SLy4 [31], in order to control that the conclusions are almost independent on the force. Because of the long range nature of the Coulomb interaction, the calculation must be started much before the turning point typically for an initial distance around 200 fm. Under these conditions a complete calculation which takes into account both nuclei would require the propagation of an enormous grid. However, since the reactions we are considering are below the barrier we can separate the dynamics of the target from the one of the projectile. Therefore, we have modify the TDHF code in order to compute the evolution of the nuclei separately in their center of mass frame. We assume that the centers of mass follow Rutherford trajectories. Since we are below the barrier, the distance of closest approach is large, and then in addition to the self-consistent potential we have only add the Coulomb field of the partner.

As an example we consider the central collision of a ^{24}Mg projectile on a ^{208}Pb target at the Coulomb barrier with the initial conditions ($\varphi_\infty = 45°$; $D_\infty = 241$ fm).

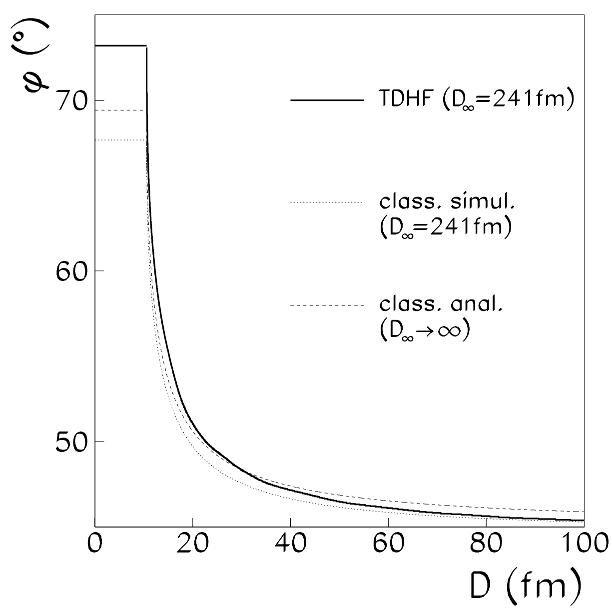

FIG. 2. For the central collision of ^{24}Mg on ^{208}Pb at the barrier the orientation φ of the ^{24}Mg as function of the relative distance D predicted by TDHF with the SkM^* force (solid line) or by classical simulation (dotted line) and its analytic approximation (dashed line).

Fig. 2 shows that the evolution of φ as function of D for classical and TDHF calculations have the same behavior. The maximum reorientation predicted by this TDHF calculation is $\Delta\varphi = 28.2°$ (resp. 33.6°), with the SkM^* (resp. SLy4) force. Both Skyrme parametrizations give the same order of magnitude ($\sim 30°$), however the classical expectation was $\Delta\varphi \sim 23°$. This 30%−difference in the reorientation indicates a smaller moment of inertia in TDHF as compared to the rigid-body classical approximation. This reduced inertia can be attributed to a spherical core in the N-body wave-function of the ^{24}Mg which does not participate to the rotation. This relative increase due to difference in the moments of inertia is independent of the initial orientation as we have numerically checked.

Experimentally, the question is: what is the effect of the reorientation on fusion cross-sections? We have used the semi-classical coupling channel code CCDEF [32] to estimate the effect of the modification of the orientation distribution at the touching point on the fusion cross-section $\sigma_{fus}(E)$ for the reaction ^{24}Mg+^{208}Pb at various energies E. The effect of reorientation are taken into account by introducing the barrier height computed for central collisions. A commonly used way to present this excitation function is to compute the so-called barrier distributions $B(E) = \partial^2_{E^2}(\sigma_{fus}(E).E)$ [33]. Fig. 3 shows barrier distributions extracted from CCDEF without shape effect (i.e. the 1D barrier, solid line). The width of the peak results from quantum tunneling. A prolate deformation $\beta_2 = 0.4$ of ^{24}Mg with an isotropic distribution of orientation (dashed line) flattens considerably the barrier distribution with a prominent part on the high energy tail. A low energy shoulder extending down to ~ 5 MeV below the 1D barrier maximum is responsible for sub-barrier fusion enhancement (as compared to the single barrier case). Classically, the low energy part of the barrier distribution can be interpreted as coming from "parallel collisions" (collision along the more elongated axis) whereas the high energy part comes from "perpendicular collisions". The high energy component dominates because a prolate nucleus has one elongated direction (low barrier) for two short axis (high barriers).

The reorientation predicted by TDHF are plotted in Fig. 3 as a dotted line. We see that the low energy shoulder is strongly reduced while the high energy peak increases. This arises from that the reorientation increases the angle between the collision and the deformation axis and thus increases the barrier height. Consequently, the sub-barrier fusion enhancement observed for reactions involving a light nucleus on a deformed heavy ion like ^{154}Sm is expected to partly disappear when the deformed nucleus is light and its collision partner heavy.

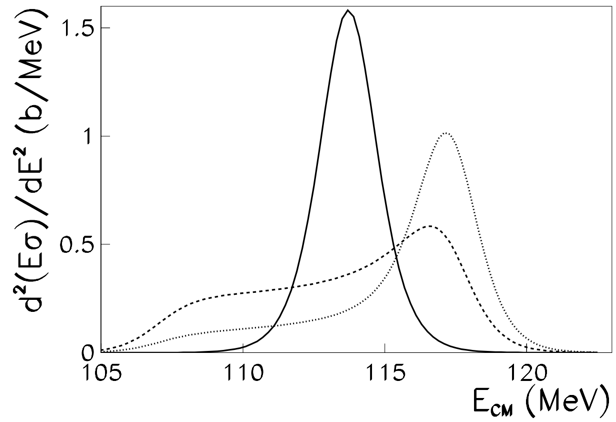

FIG. 3. Barrier distribution for the reaction ^{24}Mg+^{208}Pb obtained from CCDEF i) assuming spherical nuclei (solid line); ii) considering a prolate deformed ^{24}Mg ($\beta_2 = 0.4$) and an isotropic distribution of its orientations at the touching point (dashed line); iii) and including reorientation effects (dotted line).

Experimentally, the effect of the reorientation should be studied by comparing the excitation functions of reactions of deformed projectiles such as ^{24}Mg projectile on different target. To simplify the understanding of the reaction doubly-magic spherical targets such as ^{16}O, ^{40}Ca and ^{208}Pb might be first tested. Eq. 5 shows that the reorientation should increase with the mass of the target reducing the sub-barrier fusion, cross section.

To summarize, we have studied the reorientation effect of a deformed projectile on a spherical target. Our analytical results for the classical dynamics of a rigid body, confirmed by exact classical simulations, show that, in contrast to a naive expectation, the Coulomb reorientation depends neither on charges of both partners nor on their relative energy. The relevant observables are the deformation parameter and the masses. The reorientation is then expected to be maximum when the deformed nucleus is light and its collision partner heavy. Those conclusions have been extended to quantum dynamics using TDHF. These calculations show a sizeable increase of the reorientation as compared to classical calculations. This increase is interpreted in terms of a smaller moment of inertia for the quantum system as compared to the rigid body approximation. Calculations of barrier distributions, performed with a coupled channel code, show that sub-barrier fusion is partially hindered by the reorientation process. We finally suggest experiments to measure the effect of the reorientation on excitation functions.

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