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 its partner. This reorientation is shown to be *independent* of the charges and relative energy of the partners. It only depends upon the deformations and inertias. TDHF calculations predict an increase by 30% of the induced rotation due to quantum effects while the nuclear contribution seems negligible. 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.

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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 α radioactivity [1]. However, the tunneling of complex systems remains to be understood. As in Gamow's time, nuclear physics is providing one of the most challenging field to understand tunneling. In particular, fusion cross sections involving massive nuclei around the Coulomb barrier can be orders of magnitude over one dimensional quantum tunneling predictions. Couplings between the internal degrees of freedom and the relative motion deeply modifies tunneling [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].

For nuclei with a significant static quadrupole deformation [4,5], the main effects are i) on the barrier height (geometrical effect) since it 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 [6–10], fusion excitation functions were measured for ^{16}O (spherical) $+^{144-154}$Sm reactions. ^{144}Sm is spherical whereas ^{154}Sm is prolate ($\beta_2 \approx 0.3$). The data near the barrier were interpreted as arising from the different orientations of the prolate nucleus. An enhancement of the fusion probability is observed when the deformation axis is parallel to the collision axis (''parallel collision'') and a hindrance 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. This contradicts classical calculations [11,12] which show partial reorientation. From the quantum mechanics point of view, the reorientation is a consequence of the excitation of rotational states, which may affect near barrier fusion specially for light deformed nuclei [13,14]. Computational techniques have been developed in the past to solve coupled channel (CC) equations for Coulomb excitation [15–18] but a good understanding of the Coulomb reorientation dynamics during the approach phase is still required.

In this Letter, we obtain deeper insight in the Coulomb reorientation, reexamining the classical result, solving analytically and numerically the equations of motion of a rigid-body, and performing novel quantum approaches describing the deformed projectile within the time dependent Hartree-Fock (TDHF) theory. Then we use these reorientation results in a calculation of the fusion cross-sections. The induced effects give an helpful interpretation of full CC calculations.

Assuming first a classical treatment of nuclear orientation (the various orientations do not interfere) and ignoring any reorientation effect, the fusion cross section is given by the average orientation formula (AOF) [19,20]

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

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 looses its isotropy and the $\sin\varphi$ term in Eq. (1) has to be modified.

To estimate $\Delta\varphi$, we first consider the classical motion of a deformed rigid projectile in the Coulomb field of the target. 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 $\varepsilon = \sqrt{5/16\pi}\beta_2$, the deformation parameter.

Figure 1 shows the reorientation as function of the initial orientation for central collisions at the barrier $B = Z_p Z_t e^2/r_0(A_t^{1/3} + A_p^{1/3})$ where Z_p (A_p) and Z_t (A_t)

FIGURES

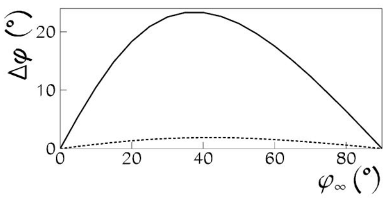

FIG. 1. Classical calculations (started at $D_\infty = 241$ fm) of the reorientation $\Delta\varphi$ of the projectile as function of its initial orientation φ_∞ for the reactions ^{24}Mg + ^{208}Pb (solid line) and ^{154}Sm + ^{16}O (dashed line) at the barrier.

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 $\varphi_\infty = 0°$ 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° whereas for ^{24}Mg it is large ($\sim 23°$).

To understand this difference, an analytical expression for the reorientation can be derived following the approximations of Ref. [21], i.e., assuming that ε and $\Delta\varphi$ are small. Computing the torque leads to following the equation of motion for $\varphi(t)$

$$\ddot{\varphi}(t) \approx \frac{9Z_pZ_te^2\varepsilon}{2mA_pD(t)^3}\sin[2\varphi(t)] \tag{2}$$

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

$$\frac{\partial\varphi(\xi)}{\partial\xi} + 2\xi(\xi - 1)\frac{\partial^2\varphi(\xi)}{\partial\xi^2} = \frac{9\varepsilon}{2\xi}\frac{A_t}{A_p + A_t}\sin(2\varphi_\infty) \tag{3}$$

where $\sin[2\varphi(t)]$ have been replaced by $\sin(2\varphi_\infty)$ treating the reorientation perturbatively (see [21]). 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 $D_0 = e^2Z_pZ_t/E$. The solution of Eq. (3) is

$$\varphi(\xi) = \varphi_\infty + \frac{3\varepsilon A_t}{A_p + A_t}\sin(2\varphi_\infty)[\xi(2 - \zeta) - \ln\zeta + \delta] \tag{4}$$

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

$$\Delta\varphi = 3\varepsilon\frac{A_t}{A_p + A_t}\sin(2\varphi_\infty)\left(\frac{1}{2} + \ln 2\right). \tag{5}$$

It can be shown by performing the time integral introduced in Ref. [22] that Eq. (5) is equivalent to the one reported in Ref. [22]. It should be noticed that Eq. (5) can be transformed in order to explicitly introduce the projectile moment of inertia $\mathcal{I}$ or equivalently the rotational excitation energy of the first excited state $E_2 = 6\hbar^2/2\mathcal{I}$. This clearly shows that in addition to a nonzero deformation, a finite $\mathcal{I}$ (i.e., a nonzero E_2) is needed to get a reorientation, i.e., a deviation from the AOF.

Equation (5) shows that the reorientation depends neither on projectile and target charges nor on the relative energy but only on the deformation and the mass ratio which is nothing but an inertia factor. This counterintuitive 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 D_0. A similar balance occurs with incident energy. An increase in E 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 $A_t/(A_p + A_t)$, and not to the Coulomb forces.

Figure 2 shows the evolution of $\varphi(D)$ for the central reaction ^{24}Mg + ^{208}Pb at the barrier with $\varphi_\infty = 45°$. 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. The difference at large distance is due to the finiteness of D_∞ (here $D_\infty = 241$ fm) in the numerical simulation while the analytical result integrates the effects from $D_\infty \to \infty$.

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 this nuclear reaction. TDHF is optimized for the prediction of the average values of one-body observables like deformation and

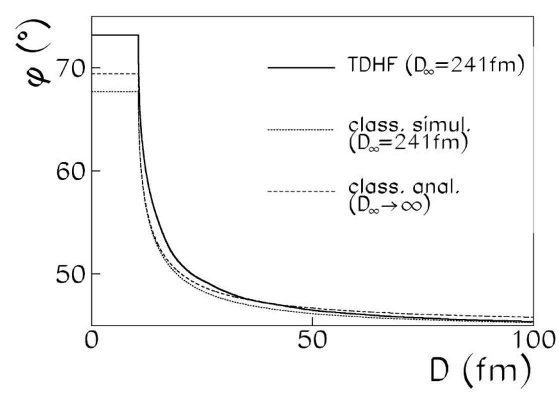

FIG. 2. For the central collision of ^{24}Mg on ^{208}Pb at the barrier the orientation φ of the ^{24}Mg as function of the relative distance D predicted by TDHF with the SkM^* force (solid line) or by classical simulation (dotted line) and its analytic approximation (dashed line).

orientation. 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, $i\hbar\partial_t\rho = [h(\rho), \rho]$ where $h(\rho)$ is the mean-field Hamiltonian. We use the code built by P. Bonche and coworkers [28] with an effective Skyrme mean field [29]. This code, which does not include pairing, computes the evolution of a Slater determinant in a 3D box. The step size of the network is 0.8fm and the step time 0.45 fm/c. 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 D_∞ around 200 fm. However, for reactions below the barrier we can separate the dynamics of the target from the one of the projectile. Therefore, we have modified the TDHF code in order to compute the evolution of the nuclei separately in their center of mass frame. The chosen box for ^{24}Mg is a cube of side size 16 fm. We assume that the centers of mass follow Rutherford trajectories and we add the Coulomb field of the partner.

The fluctuations of $\varepsilon(t)$ do not exceed 7% and then the possible excitation of vibrational modes is small and does not affect the analysis. Figure 2 shows that the evolutions of $\varphi(D)$ for classical and TDHF calculations have the same behavior. The maximum reorientation predicted by this TDHF calculation is $\Delta\varphi = 28.2°$ (33.6°), with the SkM^* (SLy4) force. Both parametrizations give the same order of magnitude ($\sim 30°$), however the classical expectation was $\Delta\varphi \sim 23°$. This 30% − difference, which is independent on the initial orientation as we have numerically checked, 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.

Experimentally, the question is: what is the effect of the reorientation on fusion cross-sections? A first qualitative investigation has been performed using the code CCDEF [32] to estimate the fusion cross-section $\sigma_{\rm fus}(E)$ for the reaction ^{24}Mg + ^{208}Pb. CCDEF takes into account the shape of the nucleus on the basis of the AOF. We then go beyond this assumption by including in CCDEF the reorientation obtained with TDHF. A commonly used way to present this excitation function is to compute the so-called barrier distribution $B(E) = \partial^2_{E^2}[\sigma_{\rm fus}(E).E]$ [33]. Figure 3(a) 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" 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).

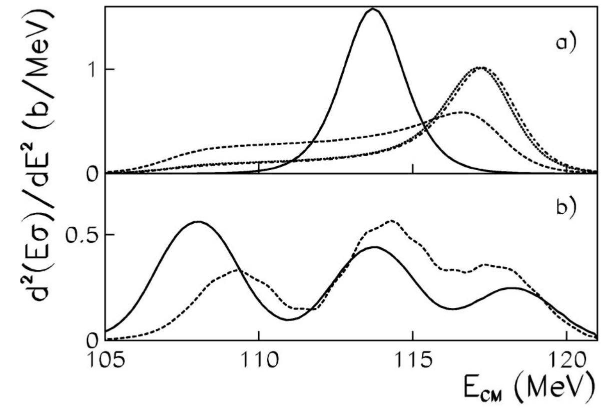

FIG. 3. Barrier distribution for the reaction ^{24}Mg + ^{208}Pb a i- assuming spherical nuclei (solid line); ii- considering a prolately deformed ^{24}Mg ($\beta_2 = 0.4$) and the AOF (dashed line); iii- and including reorientation with (dotted-dashed line) and without the rotational energy (dotted line); b) CCFULL results without (solid line) and with Coulomb coupling up to a distance of 241 fm (dashed line).

The barrier distributions including the reorientation predicted by TDHF are plotted in Fig. 3(a) both neglecting (dotted line) and taking into account the rotational energy in the trajectory (dotted-dashed line) which is a second order correction in ε and then increases only slightly the barrier. Compared to the AOF prediction the TDHF results exhibit reduced low-energy shoulder and increased high energy peak. This arises from that the Coulomb reorientation increases φ and thus increases the barrier height.

This phenomenon is implicitly taken into account in CC codes like CCFULL [34] when one uses big enough network to include long-range Coulomb couplings ($\gtrsim$ 200 fm). Figure 3(b) shows CCFULL results including nuclear (solid line) and nuclear + Coulomb (dashed line) couplings to the five first excited states of the ^{24}Mg rotational band with a long-range (241 fm). Marked variations appear in the barrier distribution due to the fact that only the lowest part of the rotational band is effectively excited [33] ($2^+ - 6^+$ in the present case). We observe, like in Fig. 3(a) a decrease of the low-energy component compensated by an increase of the high energy part of the barrier distribution. The previous TDHF+CCDEF results allow us to interpret these variations as an effect of the Coulomb reorientation.

Consequently, the sub-barrier fusion enhancement observed for reactions involving a light nucleus on a deformed heavy ion like ^{154}Sm is expected to be reduced when the deformed nucleus is light and its collision partner heavy. Experimentally, the effect of the reorientation should then be studied by comparing the excitation functions of reactions with deformed projectiles such as ^{24}Mg on different targets. To simplify the understanding of the reaction doubly-magic spherical targets such as ^{16}O, ^{40}Ca and ^{208}Pb might be first tested. Equation (5) shows that the reorientation should increase with the mass of the target reducing the sub-barrier fusion cross section.

Finally one may worry about the effect of the nuclear reorientation (implicitly included in CCFULL). We have simulated the fusion of two nuclei in TDHF. Since TDHF does not allow directly tunneling, we have studied the modulation of the threshold energy B of fusion reaction as a function of the initial orientation φ: $\Delta B(\varphi) = B(\varphi) - B(0)$. The deformed nucleus is again ^{24}Mg. To focus on the nuclear contribution we choose a light spherical target, the ^{16}O, and we start the reaction at short distance. The observed variation of B appears to follow, within the numerical error due to the considered energy step, the $\sin^2\varphi$ modulation expected for a quadrupole deformed projectile in absence of reorientation. Indeed, we get $\Delta B(45°)/\Delta B(90°) = 0.45(5)$, i.e., an almost negligible deviation from the $\sin^2$ law which predicts 1/2. Inverting the problem to extract the reorientation leads to $\Delta\varphi(45°) \sim -3°$. Considering the short range nature of the nuclear force this effect is expected to not vary much with the target. Compared with Coulomb effect this nuclear reorientation appears to be negligible. This can be related to the range of the forces. Indeed, the Coulomb interaction is a long-range force so the induced torque has time to rotate the nucleus and to produce a large reorientation which is proportional to an average angular velocity times the average time it is rotating. Conversely, the nuclear field acts over a very short time so that even if it contributes to the excitation of rotational states, the nucleus has hardly enough time to actually rotate.

To summarize, we have studied the reorientation effect of a deformed projectile on a spherical target. Analytical results for the classical dynamics of a rigid-body, confirmed by exact simulations, show that, in contrast to a naive expectation, the Coulomb reorientation depends neither on charges nor on relative energy. The relevant observables are the deformation parameter and the inertias. Those conclusions have been extended to quantum dynamics using TDHF. These calculations show that the nuclear contribution are negligible and they exhibit a sizeable increase of the reorientation as compared to classical calculations, interpreted in terms of a smaller moment of inertia for the quantum system as compared to the rigid-body approximation. The reorientation is expected to be maximum when the deformed nucleus is light and its collision partner heavy. For these systems, long-range Coulomb couplings have to be included in CC calculations of barrier distributions which show that sub-barrier fusion is partially hindered by the reorientation process. We also suggest experiments to measure the effect of the reorientation on excitation functions.

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