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TDHF studies with modern Skyrme forces

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Abstract. We present preliminary results for TDHF studies of low-energy nuclear collisions involving deformed nuclei. The computations are performed using our highly accurate 3D TDHF code, with no assumed symmetries. The code uses Basis-Splines for discretization and is written in Fortran 95.

PACS. 24.10.Cn Many-body theory – 25.70.Jj Fusion and fusion-fission reactions – 25.70.De Coulomb excitation

1 Introduction

With the ever increasing availability of radioactive ion-beams, the study of heavy-ion fusion for exotic nuclei is becoming possible. In terms of theoretical studies it is generally acknowledged that the time-dependent Hartree-Fock (TDHF) method provides a useful foundation for a fully microscopic many-body theory of low-energy heavy-ion reactions [1]. The TDHF method is most widely known in nuclear physics in the small amplitude domain, where it provides a useful description of collective states. Most of the work on large amplitude dynamics have focused on studying low energy heavy-ion collisions and relating the properties of fusion and strongly damped collisions to the properties of the effective N-N interactions. The viability of this analysis depends on the overall accuracy of the TDHF calculations. Previously, the numerical complexity and demand of extensive computer time limited studies to simple systems and employed approximations and assumptions which were not present in the basic theory. For example, most static Hartree-Fock (HF) calculations have studied the ground state properties of even-even nuclei possessing spherical symmetry, while the study of deformed systems were limited [2], whereas most TDHF calculations have been limited to cylindrical symmetry with stripped down versions of the Skyrme effective interaction.

In 1991, we have developed the world's most accurate unrestricted 3-D TDHF code with spin-orbit coupling, using B-Spline techniques [3], and applied it to fusion and deep-inelastic heavy-ion reactions. This code does not make any spatial symmetry assumptions nor does it impose time-reversal invariance for the effective interaction. Given the experimental interest in fusion of neutron-rich nuclei we have updated this TDHF code. The code has been completely rewritten taking advantage of the array processing capabilities of Fortran 95, and using the modern versions of effective interactions.

Recently, experiments have been performed at the Holifield Radioactive Ion-Beam Facility at ORNL to study fusion-evaporation residue cross-sections with neutron-rich ^{132}Sn beams on ^{64}Ni. Using this inverse-kinematics fusion technique, surprisingly large sub-barrier fusion enhancement was observed [4]. Similar experiments are planned in the future, not only at ORNL but also at other RIB facilities. In general, the heavy-ion reactions of nuclei far from stability have not been theoretically explored and pose great challenges to our microscopic approaches.

2 TDHF studies for deformed nuclei

Until today, we do not have a systematic study of TDHF collisions for deformed nuclei. This is due to the fact that if one or both of the nuclei are deformed the collision cross-sections need to be averaged over all possible orientations of the two nuclei. This is further complicated by the fact that the two nuclei approach each other on a Coulomb trajectory. This aspect is dealt with by using pure Coulomb kinematics to find out the location and the relative energy of the two nuclei at a finite separation and subsequently initializing the nuclei using these values. The two nuclei represented by Slater determinants are then boosted towards each other by a plane wave $\exp(i\mathbf{k}\cdot\mathbf{R})$ where $\mathbf{R} = \sum_i \mathbf{r}_i$, and leads to a translating solution due to the Galilean invariance of the equations of motion. However, any possible internal excitation during the Coulomb approach is ignored.

In this work, we modify the initial Coulomb kinematics to include multiple $E2/E4$ Coulomb excitation of the g.s. rotational band, since this is the primary mechanism for

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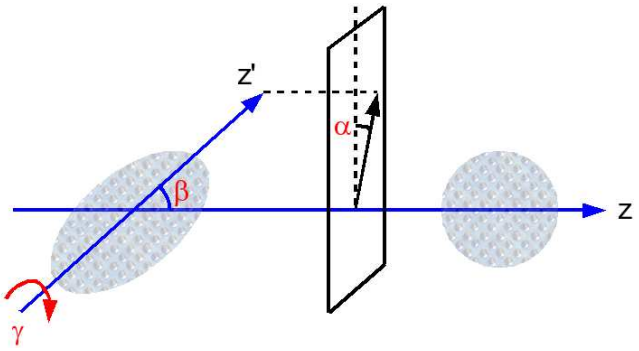

Fig. 1. Diagram showing the three Euler angles for a deformed-spherical nuclear system.

nuclear alignment during this phase. There exists an extensive literature on the "semiclassical" theory of multiple Coulomb excitation of heavy ions [5]. In this approach [6], the excitation process is described quantum mechanically, and the relative motion of the nuclei is treated by classical mechanics. The total Hamiltonian consists of the free Hamiltonian of the target nucleus, $H_0(X)$, and of the coupling potential for inelastic Coulomb excitation, $V_{\rm C}(X, \mathbf{r}(t))$. The latter depends on the intrinsic coordinates of the target (X) and on the classical relative trajectory $\mathbf{r}(t)$, and the Coulomb excitation process is determined by the time-dependent Schrödinger equation.

In the specific application of this formalism to dynamic nuclear alignment, we describe the free Hamiltonian and the corresponding wave functions in terms of the collective rotor model. The degrees of freedom are the three Euler angles $X = (\alpha, \beta, \gamma)$, depicted in fig. 1.

$$H_0(X) = T_{\rm rot}(X). \tag{1}$$

In deformed even-even nuclei, the g.s. rotational band has an intrinsic total angular momentum projection $K = 0$; therefore, the collective wave functions are independent of the Euler angle γ which describes a rotation about the intrinsic symmetry axis z'

$$\begin{aligned}\phi_r(X) &= \left(\frac{2J+1}{8\pi^2}\right)^{1/2} D^{J\,*}_{M,K=0}(\alpha,\beta,\gamma) \\ &= (2\pi)^{-1/2}\, Y_{JM}(\beta,\alpha).\end{aligned} \tag{2}$$

The probability density at time t to find the nucleus oriented with given Euler angles $X = (\alpha, \beta, \gamma)$ is given by $|\psi(X,t)|^2$; by integration over γ we find the corresponding differential orientation probability

$$\begin{aligned}\frac{{\rm d}P(\alpha,\beta;t)}{\sin\beta\,{\rm d}\beta\,{\rm d}\alpha} &= \int_0^{2\pi} {\rm d}\gamma\, |\psi(\alpha,\beta,\gamma;t)|^2 \\ &\longrightarrow \left|\sum_{J,M} a_{JM}(t) Y_{JM}(\beta,\alpha) e^{-iE_J t/\hbar}\right|^2 .\end{aligned} \tag{3}$$

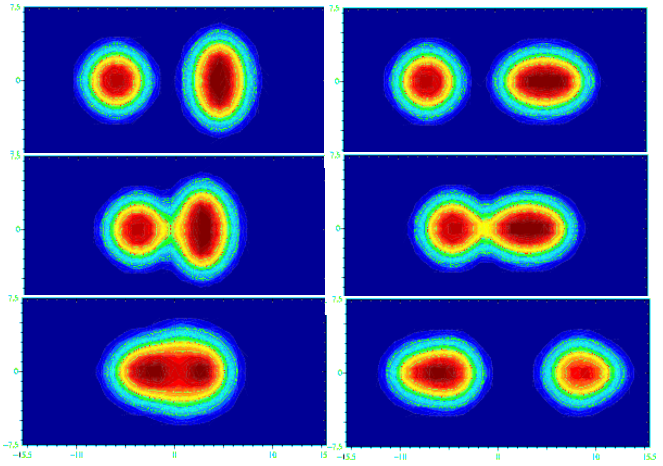

Fig. 2. TDHF collisions of ^{16}O + ^{22}Ne at $E/A = 2.5$ MeV. For the column on the left the neon is placed in perpendicular orientation, whereas in the right column the neon is horizontal. Both calculations cover a range of collisions time of about 450 fm/c. It is interesting to note that only the perpendicular configuration fuses, indicating the importance of orientation averaging.

3 Results

We have performed a number of TDHF collisions for the ^{16}O + ^{22}Ne system at a c.m. energy of 95 MeV. The two nuclei are initialized at a center-to-center separation of 16 fm and zero impact parameter (head-on). The classical Coulomb trajectory equations are solved to determine the kinematical values at this initial separation. We have used Basis-Splines of order 7, with a mesh spacing of 1.0 fm. The collision axis stretched from −16.0 fm to +16.0 fm, whereas the other two axes range from −10.0 fm to +10.0 fm. For the time spacing we have used $\Delta t = 0.2$ fm/c.

The most striking result of our calculation is the dependence of fusion on the initial orientation of the ^{22}Ne nucleus. As shown in fig. 2 when the Ne is aligned with its long axis perpendicular to the collision axis the two nuclei fuse, whereas when the alignment is horizontal to the collision axis no fusion is seen. This is an indication that the calculation of fusion needs to include a weighted average over all possible orientations as well as impact parameter. Such calculations are presently underway as well as the application of TDHF for calculating fusion cross-sections along various isotope chains.

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