Three-dimensional unrestricted time-dependent Hartree-Fock fusion calculations using the full Skyrme interaction

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We present a study of fusion cross sections using a new-generation time-dependent Hartree-Fock (TDHF) code that contains no approximations regarding collision geometry and uses the full Skyrme interaction, including all of the time-odd terms. In addition, the code uses the basis-spline collocation method for improved numerical accuracy. A comparative study of fusion cross sections for $^{16}O + ^{16}O$ is made with the older TDHF results and experiments. We present results using the modern Skyrme forces and discuss the influence of the new terms present in the interaction.

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I. INTRODUCTION

With the increasing availability of radioactive ion beams [1] the study of structure and reactions of exotic nuclei is now possible [2–4]. The microscopic description of such nuclei will lead to a better understanding of the interplay among the strong, Coulomb, and the weak interactions as well as the enhanced correlations present in these many-body systems. This has led to a considerable theoretical effort to perform nuclear structure calculations with ever-increasing accuracy and extensive investigations of the nuclear effective interaction [5].

From a theoretical point of view, these highly complex many-body systems are often described in macroscopic terms. This has been particularly true in the case of nonrelativistic heavy-ion collisions [6]. For example, the time evolution of the nuclear surface and the corresponding geometrical shape provide a very useful parameter to help organize experimental data. By using this approach numerous evolutionary models have been developed to explain particular aspects of the experimental data [7–9]. These methods provide a useful and productive means for quantifying multitudinous reaction data. In practice, they require a quantitative understanding of the data as well as a clear physical picture of the important aspects of the reaction dynamics. The depiction of the collision, including the choice of coordinates that govern the evolution of the reaction, must be given at the onset. Guessing the correct degrees of freedom is extremely hard, without a full understanding of the dynamics, and can easily lead to misbegotten results. More importantly, it is often not possible to connect these macroscopic classical parameters, describing nuclear matter under extreme excitation and rearrangement, with the more fundamental properties of the nuclear force. Ultimately, these difficulties can only be overcome with a fully microscopic theory of the collision dynamics.

In this paper, we utilize the time-dependent Hartree-Fock (TDHF) method. It is generally acknowledged that the TDHF method provides a useful foundation for a fully microscopic many-body theory of low-energy heavy-ion reactions [10–12]. The TDHF method is most widely known in nuclear physics in the small-amplitude domain, where it provides a useful description of collective states [13–15], and is based on the mean-field formalism, which has been a relatively successful approximation to the nuclear many-body problem for reproducing the principal properties of stable nuclei throughout the periodic table. During the 1970s and 1980s TDHF theory was widely used in the study of fusion excitation functions, fission, deep-inelastic scattering of heavy mass systems, and nuclear molecular resonances [10,11,16], while providing a natural foundation for many other studies. An account of some of the previous TDHF applications can be found in Refs. [10,11].

In the next section we will summarize some theoretical aspects of TDHF theory and give an account of earlier calculations as it is relevant to this work. In Sec. III we present new TDHF fusion calculations and compare them to older results and, when available, experiments.

II. THEORETICAL DETAILS

Despite the wide usage of TDHF calculations it has been difficult to assess their reliability owing to an occasional imperfect or even incorrect reproduction of experimental behavior. This has naturally led to the consideration of various extensions to the theory, particularly the inclusion of the two-body collisions [17–19]. However, there are important components of the basic theory that have not yet been fully implemented, and the viability of the analysis depends on the overall accuracy of the TDHF calculations. The assumptions and approximations that may impact the results of the TDHF calculations can be categorized as follows: (a) symmetry assumptions about the collision dynamics, (b) symmetry assumptions used for the nuclear force, and (c) accuracy of the numerical implementation. Approximations of any type limit the number of degrees of freedom accessible during a collision, and hence the nature and degree of dissipation [20–23]. The understanding of the dissipative mechanisms in the TDHF theory is vital for establishing the region of validity of the mean-field approximation and providing estimates for the importance of the mean-field effects at higher energies. In TDHF theory, the dissipation of the translational kinetic energy of the two ions is due to the collisions of single-particle states with the walls of the time-dependent potential. This leads to the randomization of the motion characterized by the distribution

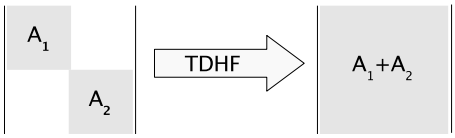

FIG. 1. Schematic illustration of the initial and final many-body states. The initial state is block diagonal whereas the final state is a full Slater determinant.

of energy among all possible degrees of freedom of the system. The complete equilibration of the translational kinetic energy among all possible degrees of freedom is commonly accepted as being the definition of fusion, whereas incomplete equilibration results in inelastic collisions.

A. TDHF collision

In TDHF calculations, the initial nuclei are calculated using the static Hartree-Fock (HF) theory. The resulting Slater determinants for each nucleus comprise the larger Slater determinant describing the colliding system during the TDHF evolution, as depicted in Fig. 1.

Nuclei are assumed to move on a pure Coulomb trajectory until the initial separation between the nuclear centers used in the TDHF evolution. Using the Coulomb trajectory we compute the relative kinetic energy at this separation and the associated translational momenta for each nucleus. The nuclei are than boosted by multiplying the HF states with

$$\Phi_j \rightarrow \exp(\imath \mathbf{k}_j \cdot \mathbf{R})\Phi_j, \tag{1}$$

where Φ_j is the HF state for nucleus j and $\mathbf{R}$ is the corresponding center-of-mass coordinate given by

$$\mathbf{R} = \frac{1}{A_j}\sum_{i=1}^{A_j} \mathbf{r}_i. \tag{2}$$

The Galilean invariance of the TDHF equations (discussed in the following) ensures the evolution of the system without spreading and conservation of the total energy for the system. In TDHF theory, the many-body state remains a Slater determinant at all times. The final state is a filled determinant, even in the case of two well-separated fragments. This phenomenon, commonly known as "cross-channel coupling," indicates that it is not possible to identify the well-separated fragments as distinct nuclei since each single-particle state will have components distributed everywhere in the numerical box. In this sense it is only possible to extract *inclusive* (averaged over all states) information from these calculations.

Approximations used in collision geometry include the assumption of an axially symmetric geometry used in earlier TDHF calculations [11]. In addition, reflection symmetry with respect to a fixed reaction plane and z-parity symmetry for identical systems have also been used. For axially symmetric calculations, noncentral collisions were studied using the so-called rotating frame approximation [24]. During the past decade some of these assumptions, especially the axial symmetry constraint, have been relaxed [25,26]. A limited number of comparisons of axially symmetric TDHF calculations with the corresponding three-dimensional calculations are available [25,27–29]. The three-dimensional calculations show more dissipation, as anticipated.

B. Effective interaction

Almost all TDHF calculations have been done using the Skyrme interaction. A variety of calculations have shown that the TDHF results are very sensitive to different parametrizations of the Skyrme force [20–23,30,31]. Fusion behavior is especially sensitive to the effective interaction [20]. Some of the assumptions made in earlier calculations included neglecting the spin-orbit force and assuming spin saturation, neglect of pairing and the use of the "filling approximation" for the occupancy of the last partially filled shell, and the time-reversal invariance of the single-particle Hamiltonian. Most of the earlier TDHF calculations also replaced some of the numerically difficult terms in the Skyrme interaction with a finite-range Yukawa form [32], without a new fit to the nuclear properties. Previously, we have shown that the inclusion of the spin-orbit interaction led to enough additional dissipation to resolve the well-known "fusion window anomaly"(a nonzero lower orbital angular momentum limit for fusion) [20–22]. Most of the new-generation TDHF programs do include at least the traditional spin-orbit interaction. However, it is well known [33] that the Skyrme energy density functional also contains terms that depend on the spin density $\mathbf{s}$, spin kinetic energy density $\mathbf{T}$, and the full spin-current pseudotensor $\overleftrightarrow{J}$ as

$$E = \int d^3r\ \mathcal{H}(\rho, \tau, \mathbf{j}, \mathbf{s}, \mathbf{T}, \overleftrightarrow{J}; \mathbf{r}). \tag{3}$$

The time-odd terms ($\mathbf{j}, \mathbf{s}, \mathbf{T}$) vanish for static calculations of even-even nuclei, whereas they are present for odd-mass nuclei, in cranking calculations, as well as in TDHF. The spin-current pseudotensor $\overleftrightarrow{J}$ is time-even and does not vanish for static calculations of even-even nuclei. However, this terms has not been commonly included in its full extent in the fitting of the Skyrme parameters owing to its numerical complexity. (The spin-orbit density $\mathbf{J}$ is the antisymmetric part of this pseudotensor and has been included.) The inclusion of these terms modifies the Skyrme energy density functional as

$$\begin{aligned}
\mathcal{H} = \mathcal{H}_0 &+ \frac{1}{4}t_0x_0\mathbf{s}^2 - \frac{1}{4}t_0\left(\mathbf{s}_n^2 + \mathbf{s}_p^2\right) + \frac{1}{24}\rho^\alpha t_3x_3\mathbf{s}^2 \\
&- \frac{1}{24}t_3\rho^\alpha\left(\mathbf{s}_n^2 + \mathbf{s}_p^2\right) + \frac{1}{32}(t_2 + 3t_1)\sum_q \mathbf{s}_q \cdot \nabla^2\mathbf{s}_q \\
&- \frac{1}{32}(t_2x_2 - 3t_1x_1)\mathbf{s} \cdot \nabla^2\mathbf{s} \\
&+ \frac{1}{8}(t_1x_1 + t_2x_2)(\mathbf{s} \cdot \mathbf{T} - \overleftrightarrow{J}^2) \\
&+ \frac{1}{8}(t_2 - t_1)\sum_q \left(\mathbf{s}_q \cdot \mathbf{T}_q - \overleftrightarrow{J}_q^2\right) \\
&- \frac{t_4}{2}\sum_{qq'}(1 + \delta_{qq'})[\mathbf{s}_q \cdot \nabla \times \mathbf{j}_{q'} + \rho_q\overleftrightarrow{\nabla} \cdot \overleftrightarrow{J}],
\end{aligned}$$

where $\mathcal{H}_0$ is the Skyrme energy density functional used in earlier calculations, with the exception of the spin-orbit term containing the density **J**. The Skyrme energy density functional does remain time-reversal invariant as all the time-odd terms enter in quadratic form or as linear bi-products. These terms, although required for TDHF theory to maintain the Galilean invariance of the collision process [34], have not been included in TDHF calculations because of numerical difficulty. Recently, because of renewed efforts toward an improved Skyrme interaction for static nuclear properties, a number of investigations have focused on identifying the importance and impact of these time-odd terms [5,34,35]. It is clear that they can no longer be neglected in TDHF calculations, at least for preserving Galilean invariance and ensuring that TDHF calculations are truly based on the same static effective interaction, since the most modern parametrization of the Skyrme force includes such terms [36]. Finally, the pairing force has sometimes been included in TDHF calculations as approximated by BCS-type pairing, where BCS equations are solved for the calculation of the initial static nuclei and the occupation numbers are kept frozen during the time evolution. It has previously been argued that, owing to the extensive continuum coupling and internal excitations during the time evolution, the effects of pairing will quickly wash away [24], whereas other calculations have shown stronger pairing correlations [37]. There is also the question of handling pairing, which is inherently related to time-reversal invariance, and the time-reversal breaking terms at the single-particle level for TDHF calculations. The study of the importance of pairing interactions during the collision process is still an open question and can only be properly answered by performing time-dependent Hartree-Fock Bogoliubov (TDHFB) calculations [38]. Finally, most Skyrme parametrizations include a one-body center-of-mass correction term, which is not included in generating the initial static solutions for the TDHF evolution.

C. Numerical approximations

From the numerical standpoint, new techniques have been developed to handle the solution of the HF equations on a space-time lattice. Equations of motion are obtained via the variation of the lattice representations of the constants of motion, such as the total energy [24,39]. In this approach, finite lattice equations that exactly preserve the constants of motion emerge from the theory in a systematic way. Most of the earlier numerical calculations have employed low-order finite-difference discretization techniques where the resulting numerical accuracies limited the studies to the gross features of the reaction. With modern supercomputers it has become feasible to carry out more extensive nuclear structure and reaction studies employing higher order discretization techniques, such as fifth- and seventh-order finite-difference techniques. Over the past decade we have developed a more modern and advanced technique by discretization of the energy density functional on a basis-spline collocation lattice, which provides a highly accurate alternative to the finite-difference method [39,40].

III. FUSION CROSS SECTIONS

Heavy-ion fusion reactions are a sensitive probe of the size, shape, and structure of atomic nuclei as well as the collision dynamics. Fusion studies using neutron-rich nuclei are becoming increasingly available. In recent experiments with heavy neutron-rich ^{132}Sn beams on ^{64}Ni [2], enhanced fusion-evaporation cross sections have been observed. Another experimental frontier is the synthesis of superheavy nuclei in cold and hot fusion reactions [41–45]. Some phenomenological models predict that the fusion cross sections depend on the heavy-ion interaction potential and on the nuclear form factors in the vicinity of the Coulomb barrier [46]. The more recent theoretical approaches for calculating heavy-ion fusion cross sections may be grouped into three major categories: (a) barrier penetration models [46–49], (b) coupled-channels calculations [50–54], and (c) microscopic many-body approaches such as the TDHF method [10,11,20,25,55].

In fusion, the relative kinetic energy in the entrance channel is entirely converted into internal excitations of a single well-defined compound nucleus. In TDHF theory the dissipation of the relative kinetic energy into internal excitations is due to the collisions of the nucleons with the "walls" of the self-consistent mean-field potential. TDHF studies demonstrate that the randomization of the single-particle motion occurs through repeated exchange of nucleons from one nucleus into the other. Consequently, the equilibration of excitations is very slow and it is sensitive to the details of the evolution of the shape of the composite system. This contrasts with most classical pictures of nuclear fusion, which generally assume near-instantaneous, isotropic equilibration. Although fusion reactions occur for light, medium, and heavy systems there are qualitative and quantitative differences among these systems. The interpretation of fusion reactions in terms of a semiclassical TDHF theory exhibits the best agreement with experiment for the lightest systems, since here fusion comprises almost the entire reaction cross section. Since TDHF is a semiclassical theory it is only possible to calculate fusion cross sections above the barrier, which is dynamically determined and may be different than the one calculated using a static two-center model. Historically, TDHF calculations have been shown to reproduce the general trends of the observed fusion data [11,25,29]. The TDHF fusion cross section is calculated using the sharp-cutoff approximation [29]

$$\sigma_f = \frac{\pi\hbar^2}{2\mu E_{\text{c.m.}}} (\ell_{\max} + 1)^2 , \tag{4}$$

where μ is the reduced mass, $E_{\text{c.m.}}$ is the initial center-of-mass energy, and the quantity $\ell_{\max}$ denotes the maximum orbital angular momentum for which fusion occurs. Previously, this expression for the fusion cross section contained a nonzero lower limit for orbital angular momentum to accommodate for central transparency observed for some systems. The so called fusion-window anomaly, which had not been experimentally seen and has been considered to be the breakdown of the mean-field approach, has been shown to disappear when the spin-orbit interaction was included in the TDHF calculations [20].

We have carried out a number of TDHF calculations for the $^{16}O + {}^{16}O$ system using different parametrizations of the Skyrme force and compared them to earlier calculations. The calculations were done in an unrestricted three-dimensional geometry using a basis-spline collocation lattice of $(-14, +14)^3$ and a lattice spacing of 1.0 fm. The static solutions were obtained using the gradient iteration method to an energy convergence of 1 part in 10^{14} and the time evolution used the exponential expansion of the infinitesimal propagator for up to 15 terms. Without assuming time-reversal invariance each single-particle state is represented by a two-spinor carrying an occupation number of $n = 1$. So, for a single ^{16}O nucleus we have 16 single-particle states, each having a spin-up and a spin-down component. The nuclei were initialized by assuming that they approach each other asymptotically on a Coulomb trajectory. The initial separation of the nuclei for TDHF calculations was taken to be 15 fm. For the criteria for fusion, we have followed the compound nuclear system long enough to observe a number of rebounds in the root-mean-square radius, as well as the disappearance of the internal two-center structure by observing the time evolution of the nuclear density. Further numerical details and the accuracy of our calculations have been discussed in Ref. [40].

We first examine the threshold energy for fusion, which is the energy above which we do not observe fusion but only inelastic collisions. This is done by performing head-on (zero impact parameter) collisions for various parametrizations of the Skyrme interaction and comparing the results to earlier TDHF calculations. It should be noted that for head-on collisions the reduction of TDHF equations to axial symmetry is almost exact. The results are tabulated in Table I along with comments indicating the details of the force selection in each case. Since the inclusion of the spin-orbit interaction was found to have a profound impact on these results [20] we do not discuss prior results that do not include this contribution. The first two threshold values denote the calculations done using axially symmetric geometry and the Yukawa finite-range approximation for the Skyrme parametrizations SkII [56] and SkM* [57]. Traditionally, all TDHF calculations included the time-odd current $\mathbf{j}$ appearing in combination $(\rho\tau - \mathbf{j}^2)$.

The next value is the same calculation performed using the exact form of the SkM* interaction and in three dimensions. As we see, the threshold energy is reduced by 8 MeV. Since axially symmetric geometry is almost exact for head-on collisions, this difference could be largely attributed to the incorrect surface behavior generated by the Yukawa approximation and perhaps to substantially improved numerical accuracy. The next four threshold values include all of the time-odd terms in the Skyrme interaction. However, there is still an unresolved issue regarding the terms containing the time-even pseudotensor $\overleftrightarrow{J}$. This term is nonzero for static calculations but has not been fully included in most fits for the Skyrme interaction. However, it may be necessary to maintain the Galilean invariance of the TDHF evolution. Repeating the same calculation for SkM* but including all of the terms in the Skyrme interaction results in a reduction of the threshold energy by another 6 MeV. Finally, we have performed calculations with more modern Skyrme forces, SLy4 and SLy5 [36]. The parametrization SLy4 does not include the $\overleftrightarrow{J}^2$ contribution to the Skyrme energy density functional. The inclusion of this term results in a 3-MeV reduction in threshold energy. This is interesting because the contribution of this term to the binding energy of the ^{16}O nucleus is on the order of a few tens of keV. The last row of Table I shows the result for the SLy5 parametrization, which includes the $\overleftrightarrow{J}^2$ contribution in determining the force parameters. We can conclude that, despite small differences, most modern forces seem to yield threshold energies that are in agreement with each other.

We have also performed fusion calculations for the $^{16}O + {}^{16}O$ system at a center-of-mass energy of 34 MeV. The reason for choosing this particular collision energy is due to the availability of older calculations and data, as well as increased sensitivity to the details of the nuclear interaction [20] for this relatively high energy collision. The results are tabulated in Table II for various parametrizations of the Skyrme force. The maximum impact parameter for fusion was searched in 1.0-fm intervals until no fusion was observed, which was then followed by a more precise search in intervals of 0.05–0.1 fm. Maximum impact parameters were found to be 6.65 and 6.60 fm for SkM* and SLy5, respectively. Again, we see substantial improvement with the more modern Skyrme forces when no approximation in geometry and interaction is used. The reduction in the total fusion cross section of 500 mb is in the right direction but still overestimates the experimental cross section [58] by about 25%. To better understand the contribution of the various new terms contained in the time-odd part of the interaction we have plotted the total energy arising from the time-odd part of the Skyrme energy density functional

TABLE I. Calculations of the fusion threshold energy for $^{16}O + {}^{16}O$ using various parametrizations of the Skyrme interaction. The subscript Y indicates that the $\nabla^2\rho$ terms are replaced by a finite-range Yukawa form for computational reasons. $\mathcal{T} = 0$ indicates that no time-reversal symmetry for the interaction was assumed.

Force	$E_{\text{threshold}}$(MeV)	Comment
SkII_Y	68	Ref. [20], 2D, only $\mathbf{j}^2$
SkM^*_Y	70	Ref. [20], 2D, only $\mathbf{j}^2$
SKM*	62	$\mathcal{T} = 0$, 3D, only $\mathbf{j}^2$
SkM*	56	$\mathcal{T} = 0$, 3D, include $\overleftrightarrow{J}^2$
Sly4	56	$\mathcal{T} = 0$, 3D
Sly4	53	$\mathcal{T} = 0$, 3D, include $\overleftrightarrow{J}^2$
Sly5	55	$\mathcal{T} = 0$, 3D, fitted with $\overleftrightarrow{J}^2$

TABLE II. Calculations of the fusion cross section for $^{16}O + {}^{16}O$ using various parametrizations of the Skyrme interaction.

Force	σ_{fusion} (mb)
SkII_Y [20]	1694
SkM^*_Y [20]	1822
SkM*	1368
Sly5	1347
Experiment	1075

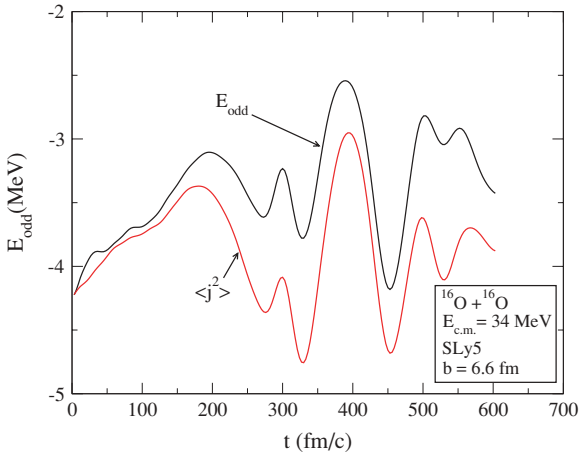

FIG. 2. (Color online) The contribution of time-odd terms to the total energy plotted as a function of time for the $^{16}O + ^{16}O$ system at $b = 6.6$ fm, using the SLy5 interaction. On the same figure we also separately show the contribution arising from the time-odd $\mathbf{j}^2$ term, which was also present in earlier TDHF calculations.

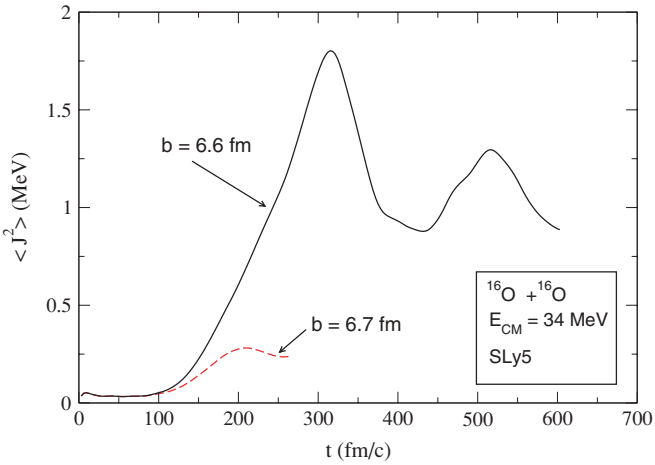

FIG. 3. (Color online) The contribution of the time-even pseudotensor term to the total energy plotted as a function of time for the $^{16}O + ^{16}O$ system at $b = 6.6$ fm and $b = 6.7$ fm, using the SLy5 interaction.

in Fig. 2. On the same figure we also separately show the contribution arising from the time-odd $\mathbf{j}^2$ term, which was present in earlier TDHF calculations. As we see, the total contribution traces the behavior of the contribution from the $\mathbf{j}^2$ term with a slight overall shift.

In Fig. 3 we plot the time evolution of the contribution to the total energy arising from the $\vec{J}^2$ term. We have plotted two impact parameters, first for $b = 6.6$ fm, where fusion occurs, and the second at $b = 6.7$ fm, where there is no fusion. We observe that when the nuclei are far apart the contribution is small and it grows as nuclei approach each other. However, we see a major difference between the case for which there is fusion and the case where no fusion occurs. In the former, the contribution rises rapidly and reaches its maximum around the time of greatest overlap during the neck formation. It then remains significant during the formation of the compound system. In the latter case the contribution remains small throughout the collision process, and finally the two fragments, albeit excited, come apart and move away from each other. This is an interesting result since this term does not seem to make a major contribution to the binding energy and does not significantly alter the parameters of the Skyrme force when it is included in the fits [36]. We can conclude from this that the nuclear properties used in fitting the parameters of the Skyrme force is not triggering the physical significance of this term.

We have repeated these calculations for the collision of ^{16}O with the neutron-rich ^{28}O nucleus at $E_{c.m.} = 43$ MeV, which maintains the same initial velocity as in the $^{16}O + ^{16}O$ case. The maximum impact parameter for fusion is found to be 7.5 fm, which results in a cross section of approximately 1767 mb. This value scales well with mass number and does not indicate an enhanced fusion cross section for this neutron-rich system. Of course, the energy is relatively high and such enhancements may be seen at lower energies or below the barrier. In Fig. 4 we show this collision for $b = 7.6$ fm, for which there is no fusion. In this deep-inelastic collision the final translational energy of the separating ions is about 20 MeV, indicating

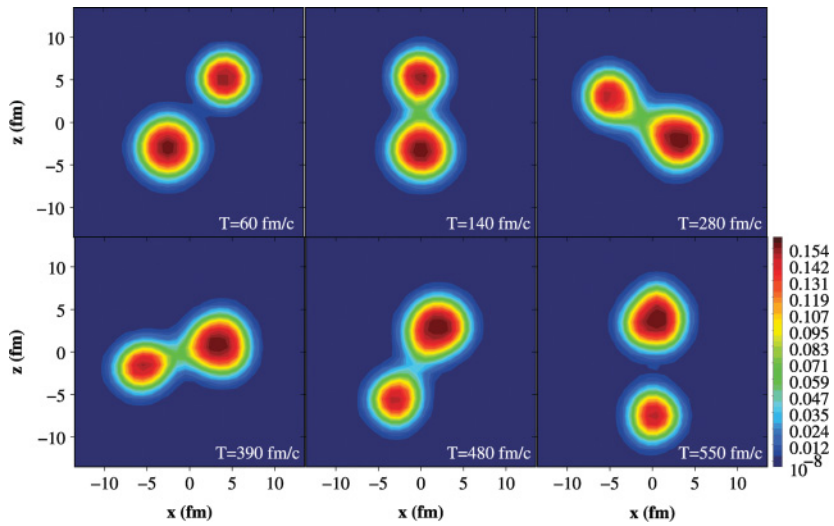

FIG. 4. (Color online) TDHF time evolution for the $^{16}O + ^{28}O$ collision at an impact parameter of $b = 7.6$ fm, just above the fusion region, using the SLy5 interaction. The initial energy is $E_{c.m.} = 43$ MeV.

that 23 MeV was utilized for internal excitations. The final fragments, besides being highly excited, show an exchange of approximately two protons and a neutron to the heavy fragment. The analysis of the various contributions arising from the terms in the Skyrme interaction shows a behavior similar to that of the $^{16}O + {}^{16}O$ system.

IV. SUMMARY AND OUTLOOK

The evolution of the TDHF studies of heavy-ion reactions is marked by increasingly sophisticated calculations, aimed at trying to eliminate as many of the assumed symmetries as possible. This progress has closely paralleled the advances in computer technology.

We have presented calculations using a new-generation TDHF program, which makes no assumptions regarding the collision geometry nor the Skyrme interaction and uses advanced numerical methods for improved accuracy. We have compared the new results with earlier TDHF calculations and analyzed the influence of the new terms in the effective interaction, specifically the new time-odd terms and the spin-current pseudotensor contribution. In general, unrestricted calculations and new Skyrme parametrizations lead to substantial improvements of fusion results. The substantially different results obtained by earlier parametrizations of the Skyrme force seem to have converged to very similar outcomes for the modern parametrizations, a sign of major strides made in improving the Skyrme interaction. Nonetheless, we find that some of the new terms make an appreciable contribution during the dynamical evolution, while being absent or minimally important for the static calculations. This suggest that improvements to the Skyrme parametrization are still possible by incorporating dynamical features into the fitting process, along the lines of Refs. [34,59]. It seems as if the mean-field approach has not yet been fully exhausted, and improved TDHF calculations may display more realistic features for heavy-ion collisions at low and medium energies.

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