The Skyrme Tensor Force in Heavy Ion Collisions

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Background: 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. The TDHF method is also known in nuclear physics in the small amplitude domain, where it provides a useful description of collective states, and is based on the mean-field formalism which has been a relatively successful approximation to the nuclear many-body problem. Currently, the TDHF theory is being widely used in the study of fusion excitation functions, fission, deep-inelastic scattering of heavy mass systems, while providing a natural foundation for many other studies.

Purpose: With the advancement of computational power it is now possible to undertake TDHF calculations without any symmetry assumptions and incorporate the major strides made by the nuclear structure community in improving the energy density functionals used in these calculations. In particular, time-odd and tensor terms in these functionals are naturally present during the dynamical evolution, while being absent or minimally important for most static calculations. The parameters of these terms are determined by the requirement of Galilean invariance or local gauge invariance but their significance for the reaction dynamics have not been fully studied. This work addresses this question with emphasis on the tensor force.

Method: The full version of the Skyrme force, including terms arising only from the Skyrme tensor force, is applied to the study of collisions within a completely symmetry-unrestricted TDHF implementation.

Results: We examine the effect on upper fusion thresholds with and without the tensor force terms and find an effect on the fusion threshold energy of the order several MeV. Details of the distribution of the energy within terms in the energy density functional is also discussed.

Conclusions: Terms in the energy density functional linked to the tensor force can play a non-negligible role in dynamic processes in nuclei.

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I. INTRODUCTION

The extent to which the time-dependent mean field is a sufficiently good description of certain phenomena in nuclear dynamics is still an open question, as evinced partly by the ongoing explorations and developments in the area [1–15]. In particular, calculations of nuclear fusion in a time-dependent Hartree-Fock framework have developed over the years with increasingly relaxed symmetry assumptions, and more sophisticated energy functionals in an attempt to settle this question. Approximations of any type limit the number of degrees of freedom accessible during a collision, and hence affect the nature and degree of dissipation. 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, 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 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 the incomplete equilibration results in inelastic collisions.

The inclusion of the spin-orbit interaction had a dramatic effect on dissipation modes in heavy-ion collisions [16, 17]. The relaxation of all spatial symmetries gave rise to yet new modes [18]. The inclusion of all time-odd terms that arise from basic (not including the extra tensor parameters) Skyrme functionals was analyzed and found to have a noticeable effect on fusion properties [19] and in giant resonances [20]. These kinds of calculations help to pin down details of the nuclear energy density functional in ways complementary to studies of nuclear matter [21–24] and of the structure of finite nuclei [25–27].

In this work, we follow up previous studies by analyzing the effect of using Skyrme functionals which include the tensor part of the original Skyrme force, and we include the most general terms in the density functional that consequently arise, noting the interesting effects that have been seen in calculations of giant resonances when adding the tensor terms [28].

In Section II we briefly outline the Skyrme force and the energy density functional used in our analysis. Section III presents TDHF calculations along with a discussion of the results, with a focus on the tensor terms of the functional. For comparison with previous work we concentrate on $^{16}$O on $^{16}$O collisions, where most of
the spin terms have no effect on the static ground state properties, so that in addition to comparison to previous studies, dynamic effects can be isolated. A concluding section (IV) follows the results.

II. THE SKYRME FORCE AND THE ENERGY DENSITY FUNCTIONAL

Skyrme’s interaction was originally posted as a zero-range low-momentum expansion of the effective interaction in nuclear medium. The original form [29] for the two-body part of the potential was given as
\[ t_{12} = \delta(r_1 - r_2) t(k', k), \]
where \( k = \frac{1}{2} i (\nabla_1 - \nabla_2) \) is the relative wave number and is placed on the right of the delta function, while \( k' \) denotes the conjugate operator placed on the left of the delta function. The potential \( t(k', k) \) was given as
\[
t(k', k) = t_0(1 + x_0 P^o) + \frac{1}{2} t_1(1 + x_1 P^o)(k'^2 + k^2) \\
+ \frac{1}{2} T(\sigma_1 \cdot k \sigma_2 \cdot k - \frac{1}{3} \sigma_1 \cdot \sigma_2 k^2 \cdot k) \\
+ \frac{1}{2} U(\sigma_1 \cdot k' \sigma_2 \cdot k - \frac{1}{3} \sigma_1 \cdot \sigma_2 k' \cdot k) \\
+ V(i(\sigma_1 + \sigma_2) \cdot k' \times k).
\]
Here, \( \sigma \) are spin matrices, \( P^o \) is the spin-exchange operator, and all other non-numeric symbols are free parameters. We note that the factor \( P^o - 4/5 \) was replaced with \( P^o \) without loss of generality in all subsequent practical usages of the interaction. In the above equation, the third and fourth lines represent the Skyrme tensor interaction, with \( T \) and \( U \) being the parameters to fit to data. In the first Hartree-Fock calculations using the Skyrme interaction, in 1972, the tensor parameters were neglected [30]. This was reasonable, since only ground states of doubly-magic nuclei were calculated. The contribution of the tensor terms is, in that case, mainly to the spin-orbit splitting, which already has an adjustable parameter (\( V \) in (1)), and the data to which the force was fitted did not demand extra parameters in the spin-orbit part.

The effect of the tensor terms was studied later, in 1977, again in doubly-magic nuclei [31], with mixed conclusions about their efficacy. Sporadically, parameter sets including tensor terms were explored, culminating in a recent resurgence in their study, motivated initially by the observed changing shell structure away from stability. The comprehensive paper by Lesinski et al., gives a summary of the history of the Skyrme tensor term, and we refer the reader there for a more complete account [25].

It is common to present the Skyrme interaction as an energy density functional. This is a more physical approach given that the original three-body force has been generalized to a density-dependent two-body term with a fractional power of the density. We adopt here the full form of the Skyrme energy density functional (EDF) as presented by Lesinski et al. [25] including all the terms which arise from the expectation value of the two-body tensor terms, following the same procedure that one uses in proceeding to the TDHF equations [32]:

\[
\mathcal{E} = \int d^3r \sum_{t=0,1} \left\{ C_t^1 [\rho_t] \rho_t^2 + C_t^0 [\rho_t] \rho_t^2 + C_t^x \rho_t \nabla^2 \rho_t \\
+ C_t^\nabla s (\nabla \cdot s) \right. \\
+ C_t^\Delta s (\nabla \cdot s) \nabla^2 s_t + C_t^\rho (\rho_t \tau_t - j_t^2) \\
+ C_t^T (s_t \cdot T_t - \sum_{\mu,\nu} J_{\mu,\nu} J_{\mu,\nu}) + C_t^F \left[ s_t \cdot F_t \\
- \frac{1}{2} \left( \sum_{\mu=x} J_{\mu,\mu} \right)^2 \frac{1}{2} \sum_{\mu,\nu} J_{\mu,\mu} J_{\mu,\nu} \right] \\
+ C_t^{\nabla J} (\rho_t \cdot J_t + s_t \cdot \nabla \times j_t) \right\},
\]
where the densities and currents are defined [25, 32, 33] in terms of the density matrix in coordinate space for protons and neutrons (indicated by the subscript \( q \)):

\[
\rho_q(r, r') = \frac{1}{2} \rho_q(r, r') \delta_{\sigma \sigma'} + \frac{1}{2} s_q(r, r') \cdot (\sigma' \langle \sigma | \sigma),
\]
with the particle density matrix being

\[
\rho_q(r, r') = \sum_{\sigma} \rho_q(r, \sigma, r' \sigma')
\]
and the spin density matrix

\[
s_q(r, r') = \sum_{\sigma \sigma'} \rho_q(r, \sigma, r' \sigma') \langle \sigma'| \sigma \rangle.
\]

The densities and currents needed are then given in terms of \( \rho_q(r, r') \) and \( s_q(r, r') \) as

\[
\rho_q(r) = \rho_q(r, r')|_{r=r'}; \\
s_q(r) = s_q(r, r')|_{r=r'}; \\
\tau_q(r) = \nabla \cdot \nabla' \rho_q(r, r')|_{r=r'}; \\
T_{q,\mu}(r) = \nabla \cdot \nabla' s_{q,\mu}(r, r')|_{r=r'}; \\
\hat{j}_q(r) = \frac{i}{2} (\nabla - \nabla') \rho_q(r, r')|_{r=r'}; \\
J_{q,\mu}(r) = \frac{i}{2} (\nabla_\mu - \nabla'_\mu) s_{q,\mu}(r, r')|_{r=r'}; \\
F_{q,\mu}(r) = \frac{1}{2} \sum_{\nu=x} (\nabla_\nu \nabla'_\mu + \nabla'_\nu \nabla_\mu) s_{q,\nu}(r, r')|_{r=r'};
\]
where the Greek letter subscripts indicate Cartesian coordinates. From these densities one then defines the isoscalar \((t = 0)\) and isovector \((t = 1)\) densities and currents found in (2) as

\[
\rho_0(r) = \rho_n(r) + \rho_p(r); \\
\rho_1(r) = \rho_n(r) - \rho_p(r),
\]

(7)
and similarly for the other densities and currents.

In the version of the energy density functional presented in (2), the contribution of the terms bilinear in the spin-current pseudotensor, \( J_t \), is presented in terms of its Cartesian components \( J_{t,\mu\nu} \). Some authors [34] use a pseudoscalar, vector and rank-2 pseudotensor representation instead. Denoting these as \( J^{(0)}_t \), \( J_t \), and \( J^{(2)}_t \) respectively, the combinations of the \( J \) pseudotensor components that appear in the energy density functional can alternatively be expressed as [25]:

\[
\sum_{\mu,\nu=x} z J_{t,\mu\nu} J_{t,\mu\nu} = \frac{1}{3} J^{(0)}_t + \frac{1}{2} J^2_t + \sum_{\mu,\nu=x} z J^{(2)}_t J^{(2)}_{t,\mu\nu}, \tag{8}
\]

\[
\frac{1}{2} \left( \sum_{\mu=x} z J_{t,\mu\nu} \right)^2 + \frac{1}{2} \sum_{\mu,\nu=x} z J_{t,\mu\nu} J_{t,\mu\nu} = \frac{2}{3} J^{(0)}_t^2 - \frac{1}{4} J^2_t + \sum_{\mu,\nu=x} z J^{(2)}_t J^{(2)}_{t,\mu\nu} \tag{9}
\]

Both of these representations are used in our work as a check of the implementation and to understand the ways in which the density functional distributes energy across different terms.

The specific EDF terms that arise only from the tensor part of the Skyrme force, that is \( C^F_s \boldsymbol{s} \cdot \boldsymbol{F} \) and \( C^{\nabla s}_s (\nabla \cdot s) \), contribute to the mean-field felt by a particle with isospin \( q \) (\( q = p, n \)) respectively through the one-body Hamiltonian operator

\[
\begin{align*}
\hat{h}^F_q &= + \sum_{q'=p,n} C^F_{qq'} \hat{\sigma} \cdot \hat{F}_{qq'} \\
&\quad - \sum_{q'=p,n} \frac{1}{2} C^F_{qq'} \left[ \nabla (s_{qq'} \cdot \nabla) + (\nabla \cdot s_{qq'}) \nabla \right] \cdot \hat{\sigma} \\
\hat{h}^s_q &= - \sum_{q'=p,n} 2C^{\nabla s}_{qq'} \nabla \cdot \hat{\sigma} \nabla \cdot s_{qq'} \tag{11}
\end{align*}
\]

where \( C^F_{qq'} = (C^F_{00} + C^F_{11})\delta_{qq'} + (C^F_{01} - C^F_{10})(1 - \delta_{qq'}) \), similarly for \( C^{\nabla s}_{qq'} \), and each of the nabla operators applies to the right hand side producing first and second order derivatives [28].

These equations complete the presentation of our Skyrme tensor implementation. The interested reader may find the remaining terms (i.e. those not solely arising from the tensor interaction) in [34], with an equivalent specification of the \((\nabla \cdot s)^2\) contribution. We note that our expression for the mean field contribution coming from the variation of the \( F \) density is expressed in a different form to that of other work (e.g. in [34, 35]), but that we have found implementing this explicitly Hermitian form to give better stability.

Full details of the mapping between Skyrme force parameterizations and energy density functional coefficients are well-documented ([34], further details can be found in [28]). We take all terms in (2), as defined by this mapping, except that we set \( C^{\nabla s}_s = C^{\Delta s}_s = 0 \), they causing instabilities, possibly related to those noted in Ref. [35]. Thus the tensor-only term given in Eq. 11 is in fact not activated in our calculations.

The inclusion of the tensor force hence brings new terms in the density functional in to play, as well as modifying the strength of pre-existing terms. We note that a recent study analyzed the effect of the tensor parameters on the spin-orbit force alone (i.e. not including the “new” terms in the functional) in the context of heavy-ion collisions [36]. One does not need to make a necessary link between the coefficients in a force representation to the coefficients of the EDF. The latter can be considered as the free parameters to be fitted to data. It is not the purpose of the present paper to produce fits to better constrain and model the effective interaction, improving its suitability for the calculations, but rather to evaluate the not yet totally explored role of the terms that arise from the tensor force, and the effect of non-zero tensor parameters on other terms in the EDF. We use existing fits from the literature, motivated as follows.

We choose SLy5 [37] as our test-bed, since there is a version of this force available which has had the tensor forces added perturbatively [38], which we denote here as SLy5t. SLy5 has also been extensively tested in TDHF collision calculations in which the full \( J^2 \) term was activated and time-odd terms studied [19]. Therefore, with this choice we are able to compare with the previous complete calculations of collisions in TDHF, albeit with no tensor force.

To test systematic properties of the tensor force parameters, we also examine the TJJ forces [25], in which the isovector and isoscalar parts of the tensor force are systematically varied, though fitted only through their contribution to the \( J^2 \) terms in the functional. Each of these forces was fitted to the same set of data and pseudodata, so give similar ground state properties in general.

We note, though, some interesting variation in static energy surface predictions among this set of forces such that different TJJ forces can yield different ground state deformations [39].
III. $^{16}$O + $^{16}$O COLLISIONS

Our calculations are performed on a Cartesian coordinate space grid with no symmetry assumptions, using a version of the Sky3D code [40] with all time-odd and tensor terms included [28, 41], except those spin-dependent terms as noted in the previous section. In the first step, the ground state of $^{16}$O is calculated with a damped gradient operator technique [42, 43]. Iterations continue until the variance in the single particle Hamiltonian is sufficiently small that the time-dependent calculation will be stable and the nucleus will translate without loss of energy on the grid [18]. We turn off any center of mass correction to be consistent between the static and dynamic calculations. Further details of the set-up of our method can be found elsewhere [41, 44].

A. Upper Fusion Thresholds for head-on collisions

The fusion window for heavy-ion collisions occurs when the nuclei have sufficient kinetic energy to overcome the Coulomb barrier, and sufficiently little that it can all be transferred to internal energy of the compound nucleus which then stays fused. Above the upper fusion threshold, the collision is deep-inelastic in nature and no fusion occurs. The fusion threshold can be rather sensitive to the choice of the energy density functional, particularly when different terms come in to play, which are not active in the ground states. We repeat previous calculations [19] for SkM*, as a check, in which it is found that activating the $J^2$ terms (which are time-even), using the standard link between the Skyrme parameters and those in (2), reduces the upper fusion threshold by 6 MeV. We reproduced the size of the reduction, but found that activating the time-odd terms (as “SkM* (full)”) increased slightly the fusion threshold, bringing it slightly closer to the “basic” SkM* force, as shown in Table I. We note, also, that the absolute values of the upper thresholds presented in [19] contained a systematic error, fixing which results in exact agreement with our results [45]. The error affected no other results presented in [19].

One sees that the tensor terms, when added to an existing parameterization (i.e. the Skyrme+tensor SLy5t compared to SLy5) can have a non-negligible effect of around 5% on the upper fusion threshold. The variation in results from the $TJ$ parameterizations is more pronounced, yielding around a 25 MeV variation in the location of the upper fusion threshold. The lower threshold in each case is determined by the Coulomb barrier, so is equal between the forces. The fusion window, therefore, can be varied widely by the tensor part of the Skyrme interaction.

<table>
<thead>
<tr>
<th>Force</th>
<th>Threshold (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SkM* (basic)</td>
<td>77</td>
</tr>
<tr>
<td>SkM* (inc. $J^2$)</td>
<td>71</td>
</tr>
<tr>
<td>SkM* (full)</td>
<td>73</td>
</tr>
<tr>
<td>SLy5 (full)</td>
<td>68</td>
</tr>
<tr>
<td>SLy5t</td>
<td>70</td>
</tr>
<tr>
<td>T12</td>
<td>61</td>
</tr>
<tr>
<td>T14</td>
<td>69</td>
</tr>
<tr>
<td>T22</td>
<td>64</td>
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<tr>
<td>T24</td>
<td>71</td>
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<td>T42</td>
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<td>T44</td>
<td>79</td>
</tr>
<tr>
<td>T46</td>
<td>87</td>
</tr>
</tbody>
</table>

TABLE I. Upper fusion threshold energies for the $^{16}$O + $^{16}$O collision using various parameterizations of the Skyrme interaction.

FIG. 1. (Color online) Contributions from terms involving some of the time-odd densities and currents to the total energy for 100 MeV collisions of $^{16}$O on $^{16}$O. Energy contributions comprise the sum of the isoscalar and isovector contributions.

B. EDF contributions in deep-inelastic collisions

We examine the contribution from different parts of the Skyrme Energy Density Functional in the regime above the upper fusion threshold, so that the collision dynamics feature a time before collision, a period where the two nuclei interact, and a subsequent period when two nuclei re-emerge with internal excitation. For $^{16}$O on $^{16}$O at 100
MeV center of mass energy we look at SLy5 and SLy5t to examine the different contribution from different terms. Figure 1 shows the contribution from the $s^2$ (split into those parts from the $I_0$ and $I_3$ parameters), the $s \cdot T$ and the $s \cdot F$ terms. Respectively, these are terms which do not depend directly on the tensor coefficients ($s^2$), are amended compared to the non-tensor case ($s \cdot T$) and only come into play with non-zero tensor parameters ($s \cdot F$).

As shown in the two upper panels of Figure 1, the $s^2$ terms begin with zero contribution, as they should with two $^{16}$O nuclei in their ground states, initialised with a Galilean velocity boost. Only when the nuclei begin to collide do these terms begin to differ from zero, as the collision process gives rise to regions of localised spin polarisation dynamically within the compound nucleus. Shortly after the collision, the $s^2$ contributions of the SLy5 and SLy5t forces do not differ, as expected since the coupling constants have not changed. Only later when the presence of the tensor terms has altered the overall dynamics do the details of the $s^2$ contributions differ between the forces, owing to changes in the $s$ density itself.

A much more evident change in the dynamics is seen in the $s \cdot T$ and $s \cdot F$ terms. Without the tensor parameters, the $s \cdot F$ term is identically zero, while it is activated with a few hundred keV of the available energy during collision via coupling to the tensor parameters. The $s \cdot T$ terms, on the other hand, have couplings combining the tensor and surface terms of the Skyrme interaction that conspire to much reduce the role of this term when the tensor terms are activated in SLy5t, compared to SLy5.

Both the terms $s \cdot T$ and $s \cdot F$ are linked by Galilean invariance to terms arising from bilinear couplings of the spin-current tensor $J_s$, as given by those terms in (2) which share the same parameter.

As a check of our approach, and also to understand the underlying dynamics and interplay between the terms in the functional, we evaluate the contributions due to the $J^2$ terms both in their Cartesian form as given in (2), and in their coupled form given in (8) and (9). Figure 2 shows these contributions. The column on the left shows the energy contributions from the (pseudo)scalar-, vector- and (pseudo)tensor-decomposed form of $J^2$ while the right hand side shows those as they appear in (2). The first three plots in the right column respectively show the contribution from the diagonal, symmetric and antisymmetric combinations of the $J$ components. The summation symbols are implicit in the figure key. As expected, the first and third terms are identically zero in the case of SLy5 since they appear only multiplied by the tensor coefficients. The bottom frames of figure 2 show the total contribution when calculated by both approaches. They are identical, as they must be.

![Figure 2](image-url) FIG. 2. (Color online) Contributions to the total energy from the $J^2$ terms following the Cartesian decomposition as in the paper by Lesinski [25] (right column) or following the coupled form given by Perlinska [34] (left column). The bottom frames show the total contribution in both cases. The case is 100 MeV collisions of $^{16}$O on $^{16}$O.

### C. Off-axis collisions

For a series of different parameterisations, we performed calculations of $^{16}$O on $^{16}$O at a center-of-mass energy of 34 MeV and impact parameter close to a grazing impact, to validate against previous work [19] for the tensor-less forces and to understand the dynamics in the nucleus. In Figure 3 we plot the contribution to the total energy of the system as described, at $b = 6.65$ fm, from the total $J^2$ terms as a function of the force parameters. It is seen that the perturbative addition of the tensor terms to the SLy5t forces results in a different sign of the $J^2$ contribution to the time-dependent mean field. The
results from the $T_{IJ}$ forces span a range of contribution, with up to several MeV of energy being stored in this term at times during the collision process. The $J^2$ terms are close to zero at $t = 0$ and they are greatly excited during the collision process. It is clear that the different behaviour of different tensor parameterisations can appear in such a dynamic situation, while being much less evident in the ground state (to which the forces are fitted). Note that this calculation shows good agreement with Figure 3 in [19], for the case of non-tensor SLy5 considered there.

We mention in this section that the impact parameter dividing those configurations which fuse from those which don’t was rather insensitive to the tensor parameter set, at least for this center of mass energy of 34 MeV. There is thus little effect on the cross-section. The study of Dai et al. [36] in which the tensor contribution to the spin-orbit interaction was evaluated, a variation in the cross-section is seen at 70.5 MeV. This is consistent with the fact that we see a reasonable spread of upper thresholds around this energy.

**IV. CONCLUSIONS**

We have performed time-dependent energy density functional calculations of heavy ion collisions using $^{16}\text{O}+^{16}\text{O}$ as a test case. We have included in the density functional all terms that arise when writing the functional from the Skyrme tensor force and used existing parameterisations to assess the effect of the tensor terms within this framework. It is found that the size of the fusion window can vary as the tensor force varies, owing to a movement in the upper fusion threshold.

Contributions from different terms in the functional were analysed. For the case where the tensor force parameters had been added perturbatively to an existing parameterisation, the largest contributions come from the $J^2$ terms. In the case of the $T_{IJ}$ non-perturbative fits, the $J^2$ terms can be of order of several MeV, though the overall variation will be affected by the general re-fit.

In the presented case of collisions of two spin-saturated nuclei, terms in the density functional which arise from the central spin-dependent and the tensor terms, play a minor role in the ground state, yet can have a significant effect in dynamical properties. Thus there may be scope for adjustment of functionals (or forces) in light of new data on dynamical processes like heavy-ion collisions while retaining simple good fits to static ground-state data. Further studies of dynamical results involving spin-unsaturated nuclei are warranted to understand the extent of the scope for adjustment.

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