TDHF FOR HEAVY IONS

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1. Introduction

Although the time-dependent Hartree-Fock (TDHF) approximation has been known for a long time [1], it has only been applied to the calculation of the behaviour of nuclei in a heavy-ion collision in the last few years. After the initial proof of feasibility and the first one-dimensional calculations [2], there was a surprisingly rapid progress in the technology of the calculations that led to a realistic two- and three-dimensional calculations, more realistic interactions and heavier systems [3-17].

At the same time, understanding about the consequences of the approximations made has deepened, and it was found that only a very limited set of physical quantities calculated in TDHF can reasonably be compared with experiment.

In this paper I shall discuss the main consequences of the TDHF approximation and the present status of comparison with experimental data. I hope that this will help to answer the question of whether the results obtained from the method are in reasonable proportion to the effort invested.

2. Derivation of TDHF

The simplest derivation of the TDHF equations involves the truncation of the equation of motion for the one-particle density matrix,

$$i\hbar \frac{\partial}{\partial t} \rho(\vec{r},\vec{r}') = -\frac{\hbar^2}{2m}(\nabla^2 - \nabla'^2)\rho(\vec{r},\vec{r}') + \int d^3 r'' \, (V(\vec{r}-\vec{r}'') - V(\vec{r}'-\vec{r}''))\rho^{(2)}(\vec{r},\vec{r}'';\vec{r}',\vec{r}''). \tag{2.1}$$

This equation still contains a general two-body interaction $V(\vec{r}-\vec{r}')$ that may, of course, be spin- and isospin-dependent, and also the two-particle density matrix $\rho^{(2)}$, in whose equation of motion in turn the three-particle density matrix appears, etc.

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The TDHF approximation may now be obtained simply by assuming the absence of two-body correlations in $\rho^{(2)}$, which in this case can be expressed in terms of ρ only

$$\rho^{(2)}(\vec{r}_1,\vec{r}_2;\vec{r}_3,\vec{r}_4) = \rho(\vec{r}_1,\vec{r}_3)\rho(\vec{r}_2,\vec{r}_4) - \rho(\vec{r}_1,\vec{r}_4)\rho(\vec{r}_2,\vec{r}_3). \tag{2.2}$$

In this case the equation (2.1) becomes self-contained and determines the time-dependence of ρ. We shall see, however, that the approximation (2.2) has far more serious consequences than is apparent at this stage.

Equation (2.1) can now be rewritten with this approximation

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \rho(\vec{r},\vec{r}') = &- \frac{\hbar^2}{2m} (\nabla^2 - \nabla'^2)\rho(\vec{r},\vec{r}') \\ &+ \bar{V}(\vec{r})\rho(\vec{r},\vec{r}') - \bar{V}(\vec{r}')\rho(\vec{r},\vec{r}') \\ &- \int d^3 r'' \, [V(\vec{r}-\vec{r}'') - V(\vec{r}'-\vec{r}'')] \\ &\times \rho(\vec{r},\vec{r}'')\rho(\vec{r}'',\vec{r}'). \end{aligned} \tag{2.3}$$

In the terms involving the two-particle interaction, we now have a direct term containing the average potential

$$\bar{V}(\vec{r}) = \int d^3 r' \, V(\vec{r},\vec{r}')\rho(\vec{r}',\vec{r}') \tag{2.4}$$

and an exchange term that is usually much too complicated to handle in a calculation. For this reason, all TDHF calculations up to now utilized some form of zero-range interaction, usually Skyrme forces, in which case the exchange term becomes similar to the direct one. The average potential in that case can be written as a functional of such quantities as the density, spin density, and so on.

Most TDHF calculations also involved additional, non-zero range, potentials like a Yukawa and a Coulomb interaction. In all of these cases the corresponding exchange contribution was neglected.

It is advantageous to express the one-particle density matrix in terms of single-particle wave functions,

$$\rho(\vec{r},\vec{r}') = \sum_{\text{occupied}} n_i \psi_i(\vec{r}) \psi_i^*(\vec{r}'). \tag{2.5}$$

n_i is unity for standard TDHF; however, in some cases, it is useful to have fractionally occupied orbits, e.g. to produce spherical ground states for non-magic nuclei ("filling approximation"). Then the system is no longer in a pure state.

Inserting Eq. (2.5) into Eq. (2.3), we get the TDHF equations in terms of the single-particle wave functions

$$i\hbar \frac{\partial}{\partial t} \psi_k(\vec{r}) = - \frac{\hbar^2}{2m} \nabla^2 \psi_k(\vec{r}) + \overline{V}(\vec{r})\psi_k(\vec{r}) - \sum_m \psi_m(\vec{r}) \int d^3 r' \, V(\vec{r}-\vec{r}')\psi_m^*(\vec{r}')\psi_k(\vec{r}') \tag{2.6}$$

where the indices k and m run over all occupied states.

At this point, one may already discuss some of the limitations of TDHF apparent from the derivation.

One trivial observation, but one that should be stressed nevertheless, is that we have a time-dependent description that involves an approximation to the change of the system at each point in time. This implies that as we let time go on our approximation will deviate arbitrarily much from the true solution no matter how good the description was during the initial stage.

Let us now discuss the approximation introduced explicitly: the omission of two-body correlations implies the complete neglect of two-body collisions during the reaction. This should be valid at low ion energies, small compared to the Fermi energy, where the Pauli principle restricts the final states available decisively and the nucleons have extremely long mean-free paths. For higher energies in the several tens of MeV per nucleon range, however, that restriction is lifted and two-body collisions may not be negligible any more. We thus have an upper limit in energy, as well as in time for the validity of TDHF.

The TDHF equations are being solved numerically by two quite different methods [7,9]. Although a comparison has shown differences between the solutions, these are very small in view of the complexity of the problem.

3. Dissipation and Thermalization

An interesting question to be asked about TDHF is to what extent it allows for a thermalization of the incoming kinetic energy.

A qualitative idea of what is happening may be obtained by examining the behaviour of the single-particle wave functions during a collision. Initially, all wave functions translate with the same uniform velocity given by the ion kinetic energy. As the collision proceeds, their translational motion becomes randomized and finally approaches something quite similar to a random thermal distribution.

The problem with this argument is, of course, that we deal with wave functions and probability distributions translating in space and not with the motion of real particles. The velocity of translation is not even observable. Still, it shows convincingly that some thermalization is going on, although we cannot determine it quantitatively as yet. The determination of a thermal energy is very difficult because quantum-mechanical uncertainties and collective motion should not be included in the thermal energy.

One further problem is that thermalization proceeds only within the space of

Slater determinants which is a very small subspace of all states accessible to the system in principle. Thus, thermalization at best corresponds to partial equilibration that will be followed by complete equilibration once all the degrees of freedom neglected in TDHF come into play.

The mechanism responsible for this equilibration is the "single-particle dissipation" proposed by Swiatecki [18]. It is the dissipation mechanism operating in a gas with mean-free path comparable to the dimensions of the system.

For the case of a heavy-ion collision, there are two idealized variants of single-particle dissipation. The "window" type describes dissipation of relative momentum of the two ions through the exchange of nucleons through the neck (or "window") joining the ions. The "wall" variant considers dissipation of kinetic energy from a moving wall that reflects the nucleons producing a net increase in their thermal energy.

There are several problems about applying these ideas to a realistic heavy-ion collision. First, it has to be assumed that there is no correlation between subsequent collisions of a nucleon with the wall or between the nucleon momenta and the wall velocity. These conditions are certainly violated e.g. for collective vibrations, and in any case the "wall" in nuclei is the average potential produced by the nucleons themselves, so that there is a correlation a priori from self-consistency. The problem of self-consistency has been investigated heuristically by Sierk, Koonin, and Nix [19] with some success, whereas Randrup and Koonin [20] tried to develop a formalism for the correlation between subsequent reflections off the wall.

An unfortunate feature of single-particle dissipation is that it is not a local effect. Because of the long mean-free path, it cannot be said where in space the corresponding thermal energy is deposited. This precludes the use of single-particle dissipation in hydrodynamical models of the microscopic type.

One may conclude from the foregoing discussion that TDHF is still the only practical method for computing single-particle dissipation in a non-idealized situation, i.e. for real heavy-ion collisions.

4. Final-State Distributions and Spurious Cross-Channel Correlations

It is in the description of the final state of a heavy-ion reaction that the restriction to a single Slater determinant is felt most strongly.

The real final state should contain all the exit channels corresponding to different angular momenta, fragment masses, fragment excited states, and so on. All of these should propagate freely towards their asymptotic limits.

In the TDHF approximation, almost all of these requirements are not fulfilled. Although TDHF contains many different breakup channels in its final states, none of these are described properly and the widths of the pertinent distributions are always found to be far too small.

Let us examine these problems in some more detail.

The initial state in TDHF is made up from two Slater determinants, one for each fragment, combined to form a larger Slater determinant for the total system. In the language of density matrices, we can write

$$\rho = \rho_1 + \rho_2 \ , \ \rho_1^2 = \rho_1 \ , \ \rho_2^2 = \rho_2 \ , \ \rho^2 = \rho \qquad (4.1)$$

where all density matrices for the combined system, as well as for each individual nucleus, are idempotent. This implies that both fragments have definite mass number.

Now if we propagate ρ in time, it will remain idempotent by virtue of the TDHF equations, but if it is dissected into a ρ_1 and a ρ_2 for the final state fragments by just cutting up configuration space, neither ρ_1 nor ρ_2 will be idempotent, so that there is a spread in fragment masses. It is found in the calculations, however, that this spread is much smaller, usually about an order of magnitude, than the experimental spreads, even if subsequent evaporation is allowed [7].

If the mass spread came out in the right order of magnitude, there would be another problem destroying confidence in the results: all of these final channels interact with each other through the average potential, an effect named "spurious cross-channel correlation" by Griffin [21]. This would certainly lead to incorrect kinetic energies and binding properties for the fragments.

It is thus advisable to accept, for the present, the narrow mass spreads in TDHF, hoping that the theory will describe the average behaviour of the reaction.

The other principal limitation to a realistic scattering theory based on TDHF is its failure to describe isolated nuclei as free particles. Nuclei remain localized indefinitely and do not spread out like wave packets in scattering theory should do. This is because although the TDHF equations are translation invariant, the non-linearity in the Hamiltonian makes all the results for the usual free particle solutions applicable to the center of mass of a TDHF nucleus.

A serious consequence of this is that the scattering angle for a given initial impact parameter and energy is precisely defined. Thus, we get essentially classical scattering behaviour from a fully quantum-mechanical theory. The classical cross sections turn out to be quite unrealistic [8].

One final problem concerns fusion especially. Although, as we saw, TDHF can incorporate a mixture of different channels in the final state, albeit unrealistically, there is never enough spread to get totally different channels -- like fusion and deep inelastic -- mixed in one collision event. Fusion will thus always be described in a sharp cut-off approximation; for each impact parameter the system fuses or does not fuse, tertium non datur.

It is clear from the above discussion that all that can reasonably be expected from TDHF is a description of the average features of the reaction, and in practice, this means fusion cross sections and the gross features of Wilczynski plots.

All of these problems and the seemingly meager area of contact with experiment should not obscure the fact, however, that TDHF has many advantages compared to other

theoretical descriptions of heavy reactions and is certainly a very worthwhile pursuit. I shall come back to a discussion of this point in the final chapter. First, though, let us examine some recent results and get an impression of the quality of results in TDHF.

5. Fusion Cross Sections and Wilczynski Plots

To give an impression of the type of agreement with experiment that can be achieved in TDHF, I here discuss some recent results of Davies et al. [22] on the $^{86}Kr + ^{139}La$ reaction.

Figures 5.1 - 5.3 show the experimental Wilczynski plots and the TDHF curve at

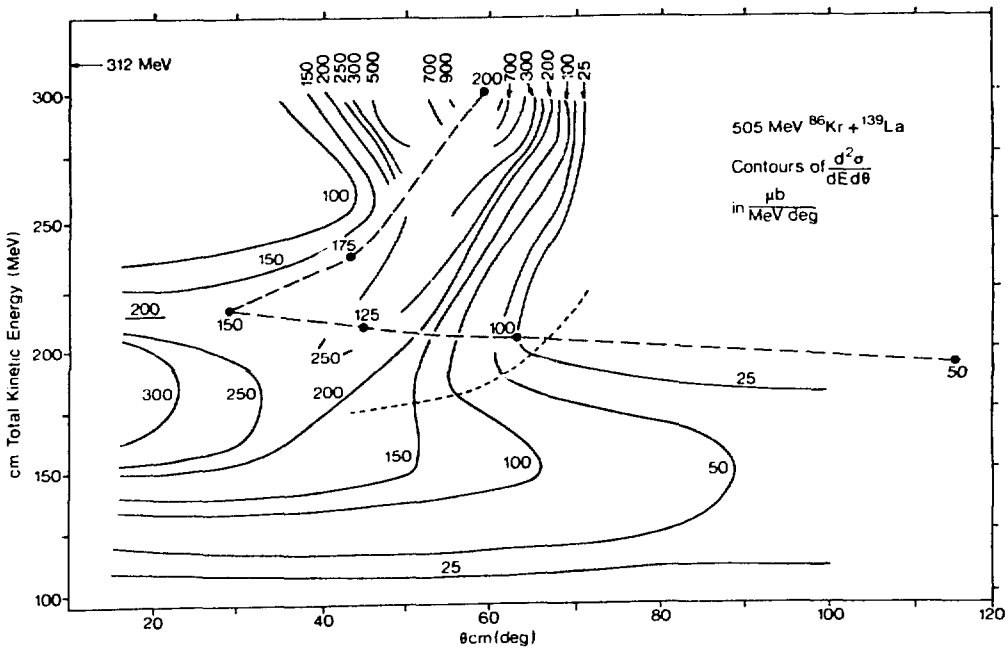

Fig. 5.1. Experimental Wilczynski plot [23] and TDHF scattering result (long dashes) for $^{86}Kr + ^{139}La$ at 505 MeV. Figure taken from Ref. [22].

three different laboratory energies. In all three cases the TDHF result reproduces the main structure of the plots quite well qualitatively, but gives insufficient energy dissipation in the deep inelastic branch. Since the calculations employed a restriction to axially symmetric shapes, there may not be sufficiently many states available, so that dissipation is reduced because of it. Still, the agreement is quite impressive considering the fact that the nucleon-nucleon interaction, in this case a full Skyrme force, is the only input to the calculations.

The spread in the final fragment masses in this case was found to be between 5 and 7 mass units, certainly quite small compared to experiment, but ensuring, on the

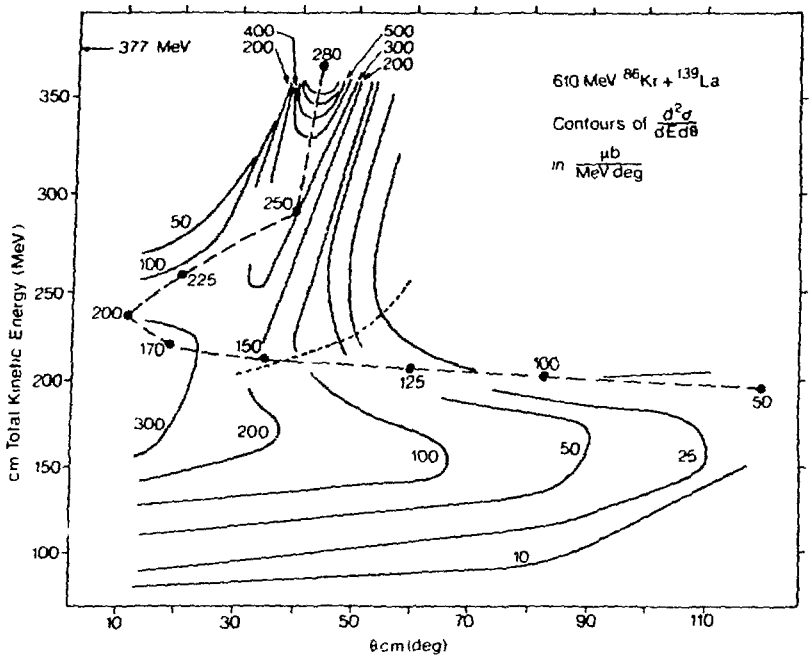

Fig. 5.2. Experimental Wilczynski plot [23] and TDHF scattering result (long dashes) for ^{86}Kr + ^{139}La at 610 MeV. Figure taken from Ref. [22].

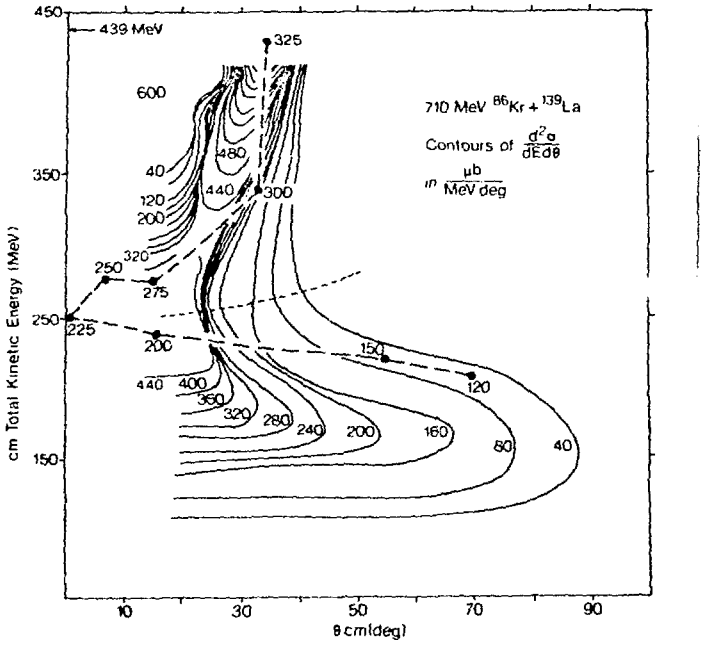

Fig. 5.3. Experimental Wilczynski plot [23] and TDHF scattering result (long dashes) for ^{86}Kr + ^{139}La at 710 MeV. Figure taken from Ref. [22].

other hand, that cross-channel correlations do not distort the results too much.

A very interesting phenomenon occurred in the fusion behaviour for this system. No fusion was observed for the two lower energies, but at the highest energy the system fused with a cross section of 118 mb. This would place the threshold for fusion between 120 and 200 MeV above the Coulomb barrier and should provide an interesting test for the TDHF method. This prediction cannot yet be asserted very strongly, though, because the insufficient dissipation seen in the Wilczynski plots may also have reduced the fusion cross section.

A more detailed study was made recently of the fusion cross sections of ^{16}O + ^{40}Ca and ^{28}Si + ^{28}Si [24]. For these, a comparison of the different types of approximations and nucleon-nucleon interactions used in various calculations was also performed. I have to refer to the original paper for a discussion of these, but I hope the different results will give an impression of the accuracy achievable at present.

Figure 5.4 shows the fusion cross section as a function of energy for ^{16}O + ^{40}Ca.

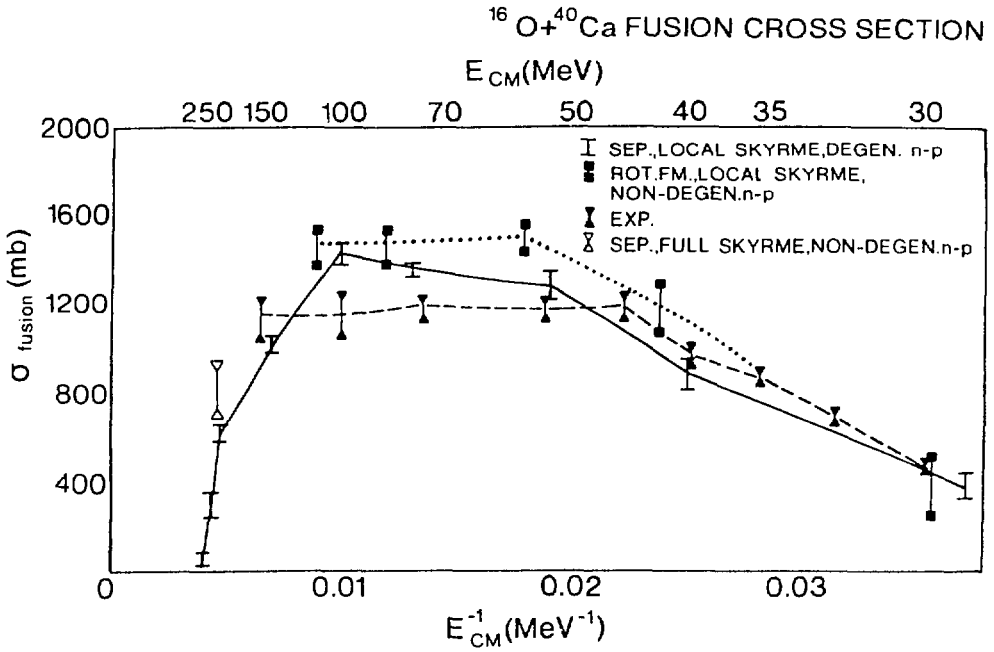

Fig. 5.4. Fusion cross section for ^{16}O + ^{40}Ca as a function of center-of-mass energy. The experimental curve [25] is compared with theoretical results obtained using various TDHF approximations. Figure taken from Ref. [24].

Apparently, all methods produce the gross behaviour quite well, but there are noticeable differences in detail, and all of them overestimate the fusion cross section at the higher energies. The difference between experimental and theoretical curves is of the same order of magnitude as that between the different theoretical ones, so

that with these calculations one should not really expect higher accuracy. It still remains to be seen whether a calculation incorporating none of the symmetry restrictions present in all of the results cited here will give more accuracy.

Figure 5.5 shows the upper and lower angular momentum limits to fusion for the

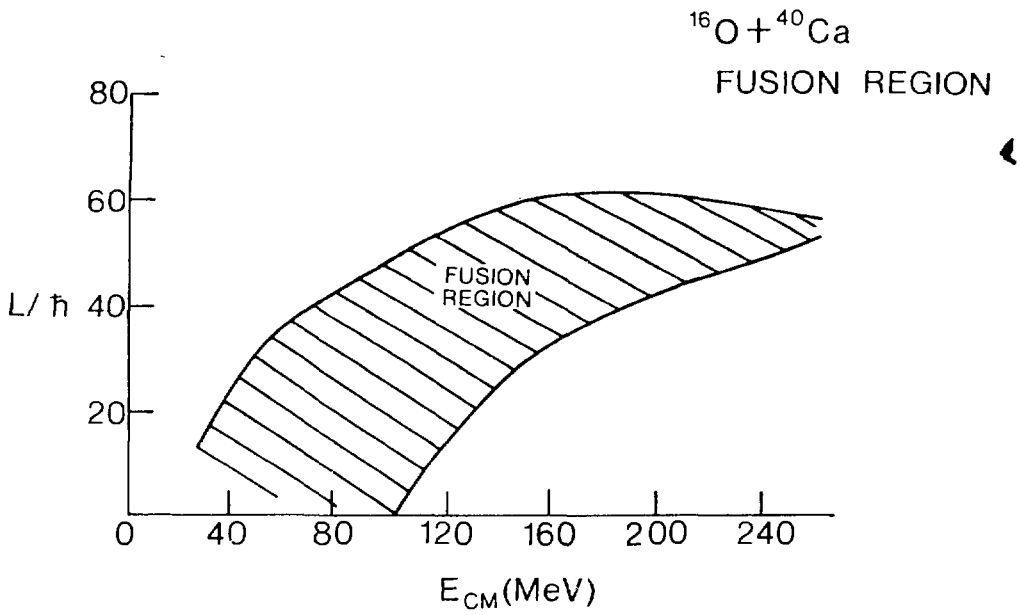

Fig. 5.5. Upper and lower angular momentum limits for fusion of $^{16}O + ^{40}Ca$, as a function of center-of-mass energy. Figure taken from Ref. [24].

same system. Above 100 MeV in the center of mass there is a fusion window, and the more rapid rise in the lower limiting angular momentum seems to be an important factor in reducing the cross section at higher energies. If that lower limit were not present, the cross section should go approximately as $1/E_{cm}$ at high energies, but in its presence the decrease is more rapid.

6. TDHF Results for a Very Heavy System

It is quite interesting to study the TDHF predictions for very heavy systems, where a closer approximation to liquid-drop behaviour is expected. Recently, calculations were carried out for the $^{238}U + ^{238}U$ system [26], and I shall here discuss some of the features appearing in those results.

Obviously, such calculations are still just barely feasible with even the fastest computers available today. Therefore, in this particular case many symmetries could not be removed. The calculation employed quartet symmetry (isospin and spin degeneracy) and a simplified Skyrme interaction, but with Yukawa and Coulomb fields included. Pairing was included in a BCS-type treatment.

Because of these restrictions, the calculations should not be regarded as representing ^{238}U nuclei realistically. They rather describe large nuclei with shell effects and pairing present. On the other hand, it is quite possible that both of these have little influence on the reaction so that the results could be applicable also to real ^{238}U nuclei.

Figure 6.1 shows a sequence of shapes for the collision at a laboratory energy of 7.5 MeV per nucleon and an angular momentum of 300ħ. We here see how after a relatively uneventful neck formation and rotation in shapes similar to the first one in this series the two nuclei separate again. There are complicated fluctuations in density inside the fragments, but these seem to correspond more to thermal fluctuations, and the really important degrees of freedom apparently are the surface shapes. But the most fascinating feature is the actual breakup of the neck. The neck becomes extremely elongated, but in the third frame the density at its center begins decreasing and this leads to a rapid snapping in the next two frames. Note that the snapping appears to start at the central region of the neck in the third frame, the lower density isolines show no constriction as yet. This is due to the equation of state of nuclear matter implied by the Skyrme force: below a certain density nuclear matter becomes unstable with respect to a further decrease in density.

The time evolution of several characteristic quantities is plotted in Fig. 6.2 for the same collision. I shall only discuss the most interesting features here:

The behaviour of the pairing gap is quite surprising. Although it decreases monotonously throughout the collision, there is still a sizable pairing gap of 0.2 MeV in the final state with about 300 MeV of excitation energy in the fragments. Whether this indicates an unexpected stability of the pairing correlations or is an artifact of the symmetries in the calculation or the BCS approximation will have to be checked in future calculations.

The orbital quantities, the separation distance and the radial kinetic energy, show an extremely smooth behaviour. Essentially this collision is dominated by Coulomb repulsion, and the neck formation and rupture are just perturbations.

The density at the center of the neck shows the characteristics discussed above; at a certain point it decreases much more rapidly than the neck radius. There is also very little compression during the collision.

Summarizing these results, one is tempted to say that a liquid-drop description using surface deformation parameters should provide a quite reasonable approximation to this reaction once the dissipative mechanisms can be inserted reliably, but the process of neck rupture certainly requires the introduction of other than mere shape coordinates.

7. Conclusions

The preceding discussion has shown that TDHF, although fraught with many intrinsic problems restricting its applicability, still provides some insight into

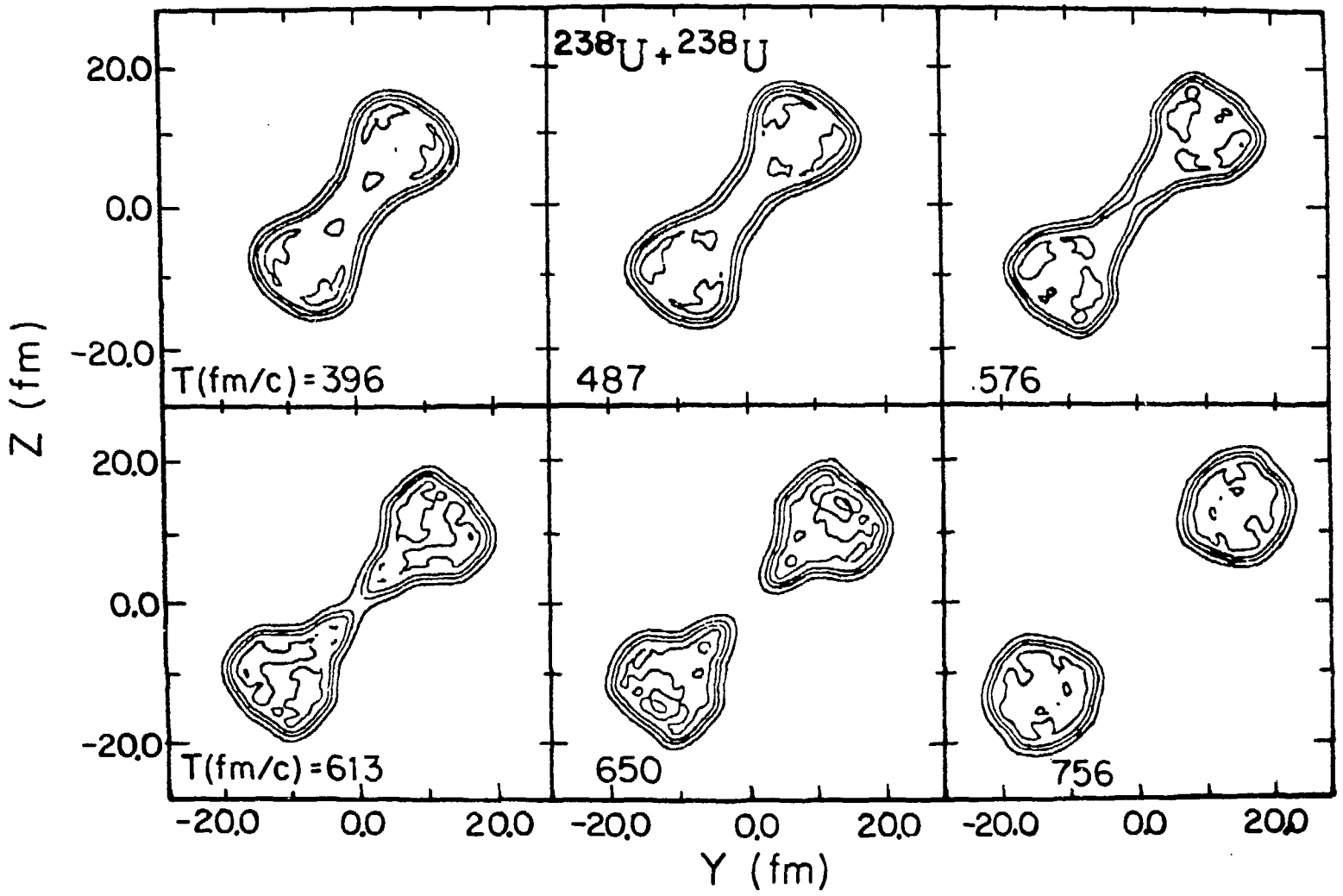

Fig. 6.1. Density distribution during the late stages of a $^{238}U + ^{238}U$ collision at 7.5 MeV per nucleon and L = 300ħ.

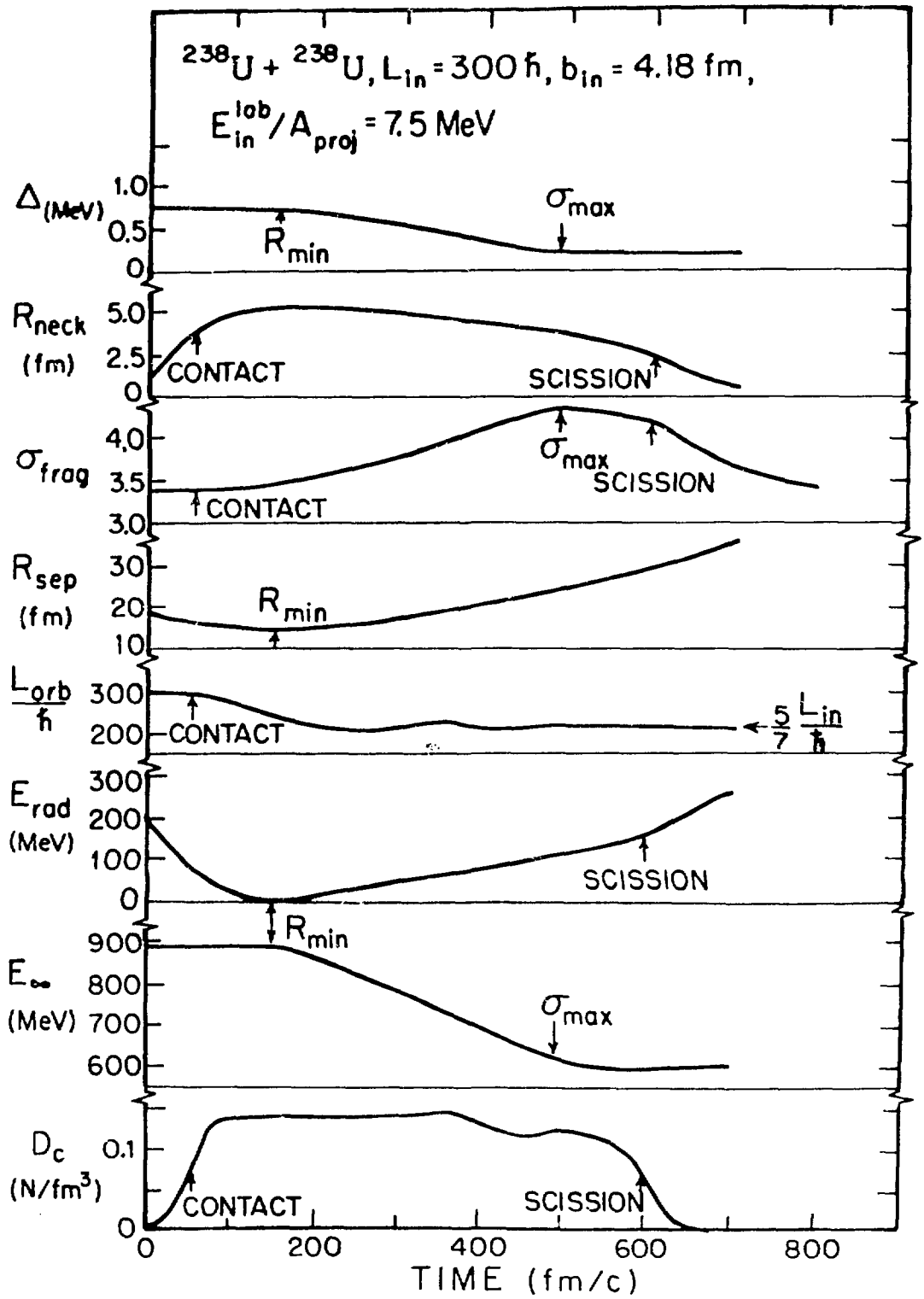

Fig. 6.2. Time dependence of various quantities during a $^{238}U + ^{238}U$ collision at 7.5 MeV per nucleon and L = 300$\hbar$. Plotted from top to bottom are the pairing gap Δ, the neck radius, the fragment deformation σ, the separation distance R_{sep}, the orbital angular momentum, the radial kinetic energy (in the c.m.), the asymptotic c.m. kinetic energy, and the density at the center of the neck.

heavy-ion collisions on a microscopic basis. Its most important advantages compared to other theoretical descriptions are the almost unlimited freedom given to the many-body system to evolve as it likes, without questionable restrictions such as frozen densities or frozen shapes, and using only the nucleon-nucleon interaction as an input. This is felt most strongly in the behaviour of the neck which, as it involves both density and surface degrees of freedom, is extremely hard to treat in more macroscopic formulations.

The fact that contact to experiment appears to be restricted to fusion cross sections and gross behaviour of Wilczynski plots is certainly a shortcoming of the method, but if these could be reproduced systematically throughout the periodic table and for a wide range of bombarding energies with just a single nucleon-nucleon interaction as input, that would certainly constitute a major achievement in understanding heavy-ion reactions.

It may be argued that the huge numerical effort is not in proportion to the results obtainable. I would counter that by stating that we should not judge the complexity of a theory by the amount of work done by the computer, but by the human effort going into it. And in this sense, once the numerical methods were understood, TDHF has become one of the simplest theories in nuclear physics, both conceptually and in practice.

TDHF can be used additionally as a starting point for considering more advanced approximations. Since these are not yet at the stage of practical application, I just refer the interested reader to the proceedings of the Paris workshop [27] for an overview.

I would like to express my gratitude to Vanderbilt University and Oak Ridge National Laboratory for their kind hospitality during my stay. Also, I am grateful to K. T. R. Davies for permission to reproduce figures from Refs. [22] and [24].

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