

Time-Dependent Hartree-Fock Theory:
Application to the $^{14}\text{N} + ^{12}\text{C}$ Reaction*

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1. Introduction

The time-dependent Hartree-Fock (TDHF) approximation to the time development of an interacting many-body system [1] has recently been investigated in its application to nuclear collisions. The progress from one-dimensional [2] to two-dimensional [3], three-dimensional with axial symmetry [4-7] and general three-dimensional [8] configurations studied was surprisingly fast in view of the computational difficulties

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involved. The astonishing flexibility present already in one-dimensional collisions [2] stimulated the expectation that TDHF might be a first step towards a really comprehensive theory of heavy-ion reactions. Soon, however, it was also recognized that TDHF is fraught with some serious interior problems which may make its direct application to experimental data difficult. The first direct comparison with experiment [7] showed some encouraging features but also serious qualitative disagreement, as will be discussed later in this paper. Therefore we use the results obtained from a "pure" TDHF calculation of the $^{14}\text{N} + ^{12}\text{C}$ reaction as the basis for further investigations designed to overcome shortcomings of the theory and leading to suggestions for further development of TDHF itself. The comparison of our final results with experimental data shows satisfactory agreement and thus demonstrates that TDHF does indeed provide a basic first step towards a more detailed theory of heavy-ion reactions.

2. Derivation of TDHF

One possible derivation of the TDHF equations, which is particularly useful for understanding the underlying physical ideas, starts from the equation for the one-particle density matrix within the BBGKY [9] hierarchy:

$$i\hbar \frac{\partial}{\partial t} \rho(r, r') = -\frac{\hbar^2}{2m} (\nabla^2 - \nabla'^2) \rho(r, r') + \int d^3r'' [v(r-r'') - v(r'-r'')] \rho^{(2)}(r, r''; r', r'') \quad (2.1)$$

Here the interaction between the particles was assumed to be expressible as an interaction potential $v(r-r')$, and $\rho^{(2)}$ is the two-particle density matrix, which can also be expressed in terms of the one-particle density matrix and a two-particle correlation function $g^{(2)}$:

$$\rho^{(2)}(r, r''; r', r'') = \rho(r, r') \rho(r'', r'') - \rho(r, r'') \rho(r'', r') + g^{(2)}(r, r''; r', r'') \quad (2.2)$$

Inserting this expression in Eq. (2.1), one obtains

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

where \bar{v} denotes the average potential,

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

On the right side of Eq. (2.3) the second term describes scattering on the average potential, followed by the corresponding exchange term, whereas the last expression denotes residual two-body interactions. In ordinary macroscopic fluid dynamics this last term has its analogy in the collision term of the Boltzmann equation; it is responsible for damping effects such as viscosity, whereas the potential scattering is usually negligible for macroscopic fluids.

In nuclear collisions, on the other hand, the average potential is strongly space- and time-dependent, while collisions are inhibited by the Pauli principle, at least at low energies.

It thus appears useful to study the approximation obtained by assuming $g^{(2)} \equiv 0$. This leads to the TDHF equation. For practical calculations, however, we have to make two further assumptions: 1) We use a zero-range density-dependent effective interaction of the simplified Skyrme type [2,9], so that the average potential becomes

$$\bar{v}(r) = -a\rho(r, r) + b\rho^2(r, r) \tag{2.5}$$

a and b are determined such as to yield an equilibrium density of $.145 \text{ fm}^{-3}$ and a binding energy of -15.85 MeV for nuclear matter. The resulting incompressibility is 368 MeV .

2) We assume a representation of $\rho(r, r')$ in terms of single -

particle wave functions of the form

$$\rho(r, r') = \sum_{\lambda} n_{\lambda} \psi_{\lambda}(r) \psi_{\lambda}^*(r') \quad (2.6)$$

with the occupation probabilities n_{λ} time-independent. This is a slight generalization of the usual single-Slater-determinant and allows partial occupation of orbitals in order to, e.g., construct spherical initial states for ^{14}N and ^{12}C in a harmonic oscillator basis. The many-body system is then not in a pure state, but this does not have any drawbacks, as all observables may be calculated via the density matrices.

The equation which is actually used in the model is thus

$$i\hbar \frac{\partial}{\partial t} \psi_{\lambda}(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi_{\lambda}(r, t) - a\rho(r, t)\psi_{\lambda}(r, t) + b\rho(r, t)^2 \psi_{\lambda}(r, t) \quad (2.7)$$

with the total density

$$\rho(r, t) = \sum_{\lambda} n_{\lambda} \psi_{\lambda}^*(r, t) \psi_{\lambda}(r, t) \quad (2.8)$$

There are as many equations (2.7) as there are n_{λ} differing from zero.

3. Numerical Solution

The equations (2.7) are solved numerically by time-stepping on a three-dimensional mesh. The integration in time is done with a predictor-corrector algorithm using the two steps

predictor: (3.1)

$$\psi(t + n\Delta t) = \psi(t + (n-1)\Delta t) + \Delta t \sum_{k=0}^{n-1} P_k^n \dot{\psi}(t + k\Delta t)$$

Corrector: (3.2)

$$\psi(t + q\Delta t) = \psi(t + (q-1)\Delta t) + \Delta t \sum_{k=1}^n C_k^{q,n} \dot{\psi}(t + k\Delta t),$$

$q = 1, \dots, n$

The quantities P_k^n and $C_k^{q,n}$ are purely numerical coefficients. Practically we found an order $n = 6$ of the algorithm optimal to achieve the accuracy discussed below at lowest cost.

The main problem in the calculation is the computation of $\dot{\psi}$ for each time, which is made difficult by the unbounded operator ∇^2 appearing in Eqs. (2.7). In order to avoid instabilities, we consider the wave functions in momentum space, which allows us to truncate undesirable high-momentum components. In momentum space the TDHF equation becomes

$$i\hbar \frac{\partial}{\partial t} \psi_\lambda(k) = - \frac{\hbar^2 k^2}{2m} \psi_\lambda(k) + \sum_{k'} \bar{v}(k-k') \psi_\lambda(k') \quad (3.3)$$

with $\bar{v}(k)$ the Fourier transform of $\bar{v}(r)$. One may eliminate the rapidly varying phase associated with the kinetic energy by setting

$$\psi_\lambda(k,t) = \phi_\lambda(k,t) \exp\left[-i \frac{\hbar^2 k^2}{2m} t\right] \quad (3.4)$$

so that the equation (3.3) becomes

$$i\hbar \frac{\partial}{\partial t} \phi_\lambda(k,t) = \sum_{k'} \bar{v}(k-k') \phi(k',t) \exp\left[i \frac{\hbar^2}{2m} (k^2 - k'^2) t\right] \quad (3.5)$$

Stability is further enhanced by truncating those components of the wave function for which

$$\hbar^2 k^2 / 2m > E_{cut} \quad (3.6)$$

For the collision energies considered, $E_{cut} = 125$ MeV gave sufficiently accurate results.

The entire calculation cannot, however, be carried out in momentum space, because folding with the potential \bar{v} is too time-consuming. Therefore we introduce a coordinate mesh

$$r_{klm} = (k \cdot \Delta x, l \cdot \Delta y, m \cdot \Delta z) \quad (3.7)$$

and a corresponding momentum mesh

$$k_{rst} = 2\pi \left(\frac{r}{N_x \Delta x}, \frac{s}{N_y \Delta y}, \frac{t}{N_z \Delta z} \right) \quad (3.8)$$

with $k, r = 1, \dots, N_x$; $\ell, s = 1, \dots, N_y$; $m, t = 1, \dots, N_z$.

Functions can be transformed back and forth via the finite Fourier expansion, which can be done extremely rapidly using the Fast-Fourier-Transform Algorithm [10, 11]. Thus the potential operator is actually applied on the wave function in coordinate space, where it is diagonal, and the result is transformed back into momentum space.

In the calculation we put $\Delta x = \Delta y = \Delta z = 1$ fm; $N_x = 16$, $N_y = 24$, $N_z = 24$ (the x-axis perpendicular to the scattering plane), and for a maximum stable timestep of 1.25 fm/c total energy was conserved within 0.5 MeV and the sum of the norms of the wave functions to within 10^{-5} . The latter is a particularly stringent test as our algorithm is not explicitly unitary.

The symmetries assumed for the system were 1) quartet symmetry, i.e. neglect of spin- and isospin differences; 2) Reflection symmetry about the scattering plane; and 3) (for collisions with equal mass of projectile and target only) inversion symmetry.

For the initial conditions we used harmonic oscillator wave functions with the occupation of the 1 p shell such as to produce spherical ground state density distributions. The centers of mass of the ^{12}C and ^{14}N distributions were set 10 fm apart, and the wave functions for the two clusters were multiplied with the appropriate phase factors $\exp[\pm i k_0 r]$, with the vector k_0 depending on the energy and impact parameter.

The calculation also contained the Coulomb interaction, which for simplicity was suppressed for the discussion in chapter 2. The exchange contribution had to be neglected, however. For large impact parameters in the pure Coulomb scattering regime we could reproduce the scattering angles within 1%.

4. Results of Pure TDHF

The results of the pure TDHF theory as discussed up to now show the complete development of the wave functions during the collision. Each collision is determined completely by the incident energy and impact parameter. Since details of their time dependence will be shown later in this conference [12], only an overview of the results will be given here.

For a light system like $^{14}\text{N} + ^{12}\text{C}$ we may distinguish roughly four different types of scattering occurring for different ranges of the impact parameter. At very large impact parameters, outside the range of nuclear forces, we get only Coulomb scattering. In the next smaller range the trajectories are bent back by nuclear forces. There then is a small range of impact parameters for which the attractive and repulsive forces balance such as to let the two nuclei orbit around each other for an extended period, i.e. for one or even several revolutions. Finally for small impact parameters around the central collisions the nuclei come out of the interaction at 0° (because of antisymmetry, no statement can be made about whether the nucleons or clusters really "pass through" or are exchanged, however, in asymmetric collisions the nucleus ejected in the forward direction has an average mass quite close to that of the projectile, so that in this sense one may speak of the projectile "passing through" the target).

The final kinetic energy of the two fragments can be determined from the translational motion of their centers-of-mass in the final state, and this may be extrapolated to infinity with a Coulomb trajectory, in the same way as the initial is propagated to a distance of 10 fm from infinity.

Although the interaction of the two nuclei, which gives rise to the final state, is a very complicated quantum-mechanical process, the final state itself can be used only in a classical scattering formalism. The reason is that the center-of-mass of each nucleus is not free, but is also bound with roughly constant localization, so that asymptotically the

uncertainty in angle goes to zero and there are no interference effects. Thus the only information to be obtained classically are the final scattering angle θ_f and final kinetic energy E_f as functions of the incident energy E_i and impact parameter b .

For fixed E_i the differential cross section may be calculated from the classical formula

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} \left\{ \frac{d(\cos \theta_f)}{d(b^2)} \right\} \quad (4.1)$$

Evaluations using this formula were done by V. Maruhn-Rezwani et al. [7]. Although these were based on an axially-symmetric TDHF calculation, the differences to our results should only be quantitative. The result is a cross section that decreases as $\sin^{-1}\theta_f$ for small angles, in contrast to the experimentally observed exponential decrease [15].

Another severe difference to experiment is the low probability for fusion in TDHF, if fusion is defined by a very long lifetime of the compound system with respect to break-up. The main deexcitation process leading to fusion, namely particle evaporation, has not been seen in TDHF calculations yet. A simple solution consists of selecting a time limit that indicates the reliability of TDHF; if the compound system lives longer, it is assumed, decay processes such as evaporation, which are not included in the calculation, will take over and allow it to settle down [7, 12]. Since this method defines the fusion cross section uniquely only if there is a very abrupt change in interaction time as a function of impact parameter, a more detailed treatment is clearly required. In the next two sections we shall give a simple heuristic procedure to correct both, fusion and center-of-mass problem. It should be stated clearly, however, that these additions are not part of pure TDHF.

The possibly most severe problem associated with TDHF, viz. the unrealistic description of the outgoing channels and their spurious interactions, is not treated in this paper. It is not believed to be detrimental to the present calculations, as for

these light systems the mass spreads were found to be quite small ($\lesssim 2$ mass units), and this should be indicative of other quantum numbers as well.

5. The Scattering Amplitude

The unrealistic description of the center-of-mass motion of the fragments in TDHF suggests supplementing the TDHF calculation by using the TDHF results only during the interaction itself and replacing the motion of the separated fragments with that of free wave packets. During the short interaction time the lack of spreading should not be severe unless we are dealing with very low energies.

Thus we assume that the incoming wave can be expanded in TDHF wave packets centered around an impact parameter b (other quantum numbers suppressed):

$$\psi^{in} \approx \sum_b c_b \psi_b^{in} \quad (5.1)$$

The wave packet ψ_b is then propagated in time by the rules of TDHF and will reach a final state

$$\psi_b^{out} = f_b(\theta) \phi^{out} \quad (5.2)$$

where ϕ^{out} is an outgoing wave packet and $f_b(\theta)$ a function peaked around $\theta = \theta_f(b)$. The scattering amplitude will then be given by

$$f(\theta) = \sum_b c_b f_b(\theta) \quad (5.3)$$

The preceding discussion is only a sketch of a mathematical treatment of the problem. The steps are by no means proved nor will it be easy to do so, as the TDHF equations are nonlinear and the superposition principle thus does not hold for TDHF wave packets.

However, it appears physically reasonable that a theory along these lines could be constructed. For the present we take recourse to a result of semiclassical scattering

theory [14, 15], which expresses the phase shifts directly in terms of the deflection function

$$\delta_\ell \simeq -\frac{1}{2} \int_{\ell+\frac{1}{2}}^{\infty} \Theta_f(\ell) d\ell \quad (5.4)$$

The angular momentum is related to the impact parameter via

$$\ell = A_1 A_2 b \sqrt{\frac{2}{m} \frac{E_f}{A_p}} (A_1 + A_2)^{-1} \quad (5.5)$$

with the subscript "p" denoting the projectile.

Each outgoing wave packet has a different expectation value of the kinetic energy, so that it appears that in TDHF wave packets for different ℓ -values do not interfere. However, at the end of the collision the wave functions are strongly time-dependent, so that they have a considerable energy spread. Estimating its size from the time needed to break up the neck, which is the dominant time-dependence, we arrive at a value of $\Gamma = 20$ MeV, which is used in all further calculations. (The results did not seem to be sensitive to this parameter, at any rate). We thus spread the final state in energy with a factor

$$g_\ell(E) = (\Gamma\sqrt{\pi})^{-\frac{1}{2}} \exp\left[-(E - E_f(\ell))^2 / 2\Gamma^2\right] \quad (5.6)$$

The semi-quantal reaction amplitude now takes the form

$$f(\theta) = -\frac{i}{2} \sum_{\ell} \frac{(2\ell+1)}{k} g_\ell(E) c_\ell e^{2i\delta_\ell} P_\ell(\cos\theta) \quad (5.7)$$

is the probability amplitude for the system to emerge in this channel, e.g. in this case we are looking at direct inelastic scattering and if fusion is considered to be the only other channel, then c_ℓ^2 gives the probability for not fusing. The fusion cross section is then given by

$$\sigma_{\text{fusion}} = \frac{\pi}{k_i^2} \sum_{\ell} (2\ell+1) (1 - c_\ell^2) \quad (5.8)$$

The method used to determine the C_e is given in the next section.

6. The Fusion Probability

The TDHF theory contains a thermal excitation of the nucleonic degrees of freedom by a randomization of nucleon motion via collisions with the moving walls. Our basic assumption now is that this thermal excitation may lead to nucleon evaporation and that once a nucleon is evaporated the system has lost so much energy that it will fuse. Implicitly it is also assumed that nucleon evaporation is the dominant de-excitation process during the collision, but that should be quite well fulfilled.

We define the thermal energy as

$$E_{th}(t) = E_{tot} - E_{coll}(t) - E_{fermi}(t) \quad (6.1)$$

Here E_{tot} is the (constant) expectation value of the Hamiltonian and E_{coll} is the energy of collective motion defined in analogy with fluid dynamics

$$E_{coll}(t) = \frac{1}{2} m \int d^3r j^2(r,t) / \rho(r,t) \quad (6.2)$$

$j(r,t)$ is the total local flow of probability for finding a nucleon, and $\rho(r,t)$ is the probability density for nucleons (same as (2.5)). The "Fermi energy" E_{fermi} finally gives the energy contained in the Fermi motions of the nucleons for the ground state. We approximate it with a Thomas-Fermi-expression [15]

$$E_{fermi} = \int d^3r [A \rho(r)^{5/3} + B |\nabla \sqrt{\rho}|^2] \quad (6.3)$$

where A is a numerical constant and B is adjusted so that at the beginning of the collision we get $E_{th} = 0$.

The thermal energy obtained in this way is then inserted into an expression for the evaporation width of an excited

nucleus [19]

$$\Gamma(u) = c R^2 \frac{A-1}{A} \left(\frac{u-u_0}{a} \right) \left(\frac{u}{u-u_0} \right)^{3/4} \times \exp \left[2\sqrt{a} (\sqrt{u-u_0} - \sqrt{u}) \right] \quad (6.4)$$

Here $U_0 \approx 8$ MeV is the evaporation threshold, $c = 0.0153$, $R = 1.2 (1+(A-1)^{1/3})$, and U is the sum of thermal and rotational energy. The angular momentum dependence of the width as given in Ref. 19 was found to be negligible. Since Γ depends on time via U , the total probability for evaporating a nucleon during one collision is determined by

$$1 - C_\ell^2 = 1 - \exp \left[-\frac{1}{\hbar} \int_{t_i}^{t_f} dt \Gamma(u(t)) \right] \quad (6.5)$$

C_ℓ^2 gives the probability for staying in the direct inelastic channel. Identifying $1 - C_\ell^2$ with the probability for fusion is a further assumption that takes evaporation to be the dominant decay mode and assumes that one evaporation suffices to let the system fuse.

The fusion cross section is now given by

$$\sigma_{\text{fusion}} = \frac{\pi}{k_i^2} \sum_{\ell=0}^{\infty} (2\ell+1)(1-C_\ell^2) \quad (6.6)$$

7. Results

In the following we shall discuss data calculated for the $^{14}\text{N} + ^{12}\text{C}$ reaction at 8 MeV per nucleon in the lab system.

Fig. 1 shows the classical deflection function obtained from TDHF. One may clearly discern the pure Coulomb scattering above $\ell = 28$. For smaller ℓ -values the angle becomes negative and quite large around $\ell = 15$, going back gradually

to zero for the near-central collisions.

Fig. 2 contains the angular-momentum dependence of the total kinetic energy loss and the amplitude for remaining in the direct inelastic channel as discussed in section 6. The energy loss increases monotonously for decreasing ℓ , with the steepest part of the curve associated with angular momenta slightly below the grazing value. It is important to note, however, that the biggest energy loss occurs for the central collisions, although these have a relatively short interaction time. The amplitude curve shows that there is complete dominance of fusion only for the "orbiting" angular momenta.

The fusion cross section computed from these data is $\sigma = 856 \text{ mb}$, in good quantitative agreement with the experimental value of $900 \pm 100 \text{ mb}$ [16].

The doubly differential cross section $d^2\sigma/d\Omega dE$ is plotted in a three-dimensional representation in Fig. 3 to show the structure more clearly, the curves have been cut off at 400 mb/MeV sr .

The peak at high energies and small angles arises mainly from ℓ -values above the orbiting value, whereas the low energy small angle peak is caused by the "feed-through" scattering at small ℓ . Experimentally, the energy loss in this region is so large that the fragments cannot be distinguished from fusion residues. Comparison with experiment therefore has to concentrate on the high-energy peak. By integrating the cross section from 50 MeV upward in energy we get the angle-dependence of the cross section for direct inelastic scattering, which is compared to the experimental cross section [13] in Fig. 4. The theoretical curve now shows an exponential fall-off as does the experimental one, but it still contains pronounced oscillations at forward angles due to Fraunhofer scattering. This effect may vanish if we take the hitherto neglected distribution of the final spins of the fragments into account. The overall normalization of the theoretical curve is off by about a factor of three, but this turned out to depend sensitively on the precise values of the

fusion probability, so that one will have to be content with the present situation until a more rigorous treatment has been devised for these.

The dashed curve in Fig. 4 shows the cross section integrated in energy from 0 to 50 MeV, i.e. for the small angular momenta "feed-through" scattering. No comparison to experiment is possible for this curve at present.

In order to check the dependence of the results on the presence or absence of this type of scattering, we artificially suppressed it by setting $C_\ell=0$ for ℓ less than the orbiting value. The result is shown in Fig. 5. There is still some residual cross section between 0 and 50 MeV, but it is less by more than a factor of ten. It is interesting to note, however, that the direct inelastic cross section is affected only in the details of the oscillations at larger angles, so that this type of measurement is not sensitive to such a cut off. The fusion cross section is increased to about 1055 mb for this case and is thus somewhat larger than the experimental value.

8. Conclusion

The results discussed above show that the TDHF theory contains many of the features needed for a fundamental description of heavy-ion reactions, but has serious deficiencies as well. The variety of scattering events at different impact parameters show the flexibility of the theory, and the substantial energy losses suffered in the collisions appear to indicate that single-particle viscosity is indeed a strong, and possibly the dominant, dissipative mechanism for heavy ions at the energies considered [17]. The heuristic solutions we have presented for the center-of-mass motion and fusion problems are certainly not definitive, but we hope that they indicate the directions in which the theory will have to be expanded: The combination of TDHF with a rigorous scattering theory is essential to obtain results which go beyond classical behaviour. In order to treat fusion, and in general the

presence of distinct channels, more realistically, however, one will have to go beyond the single-Slater-determinant approximation. Since this may destroy the one supreme attractive feature of TDHF - namely its computability -, one may have to study these generalizations in one-dimensional situations.

Acknowledgements

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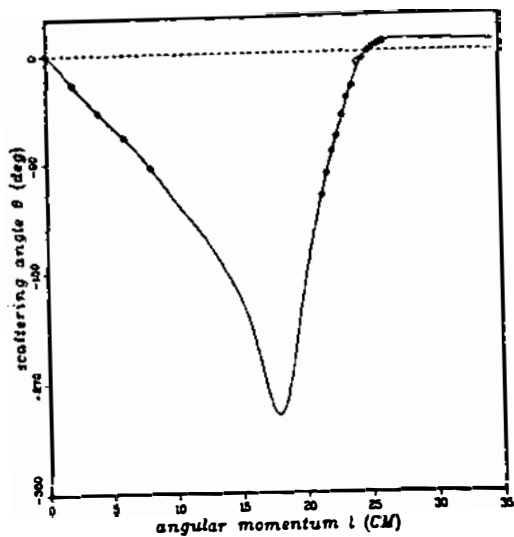


Fig. 1.

The TDEF deflection function for $^{14}\text{N} + ^{12}\text{C}$ at 8 MeV per nucleon in the lab system.

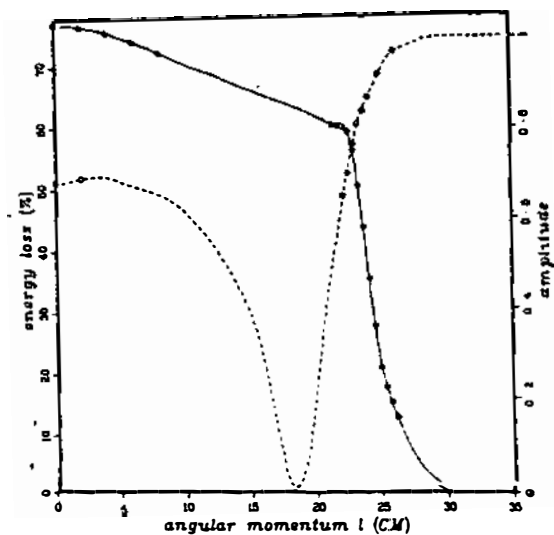


Fig. 2.

Energy loss (solid curve) and direct inelastic amplitude as functions of angular momentum.

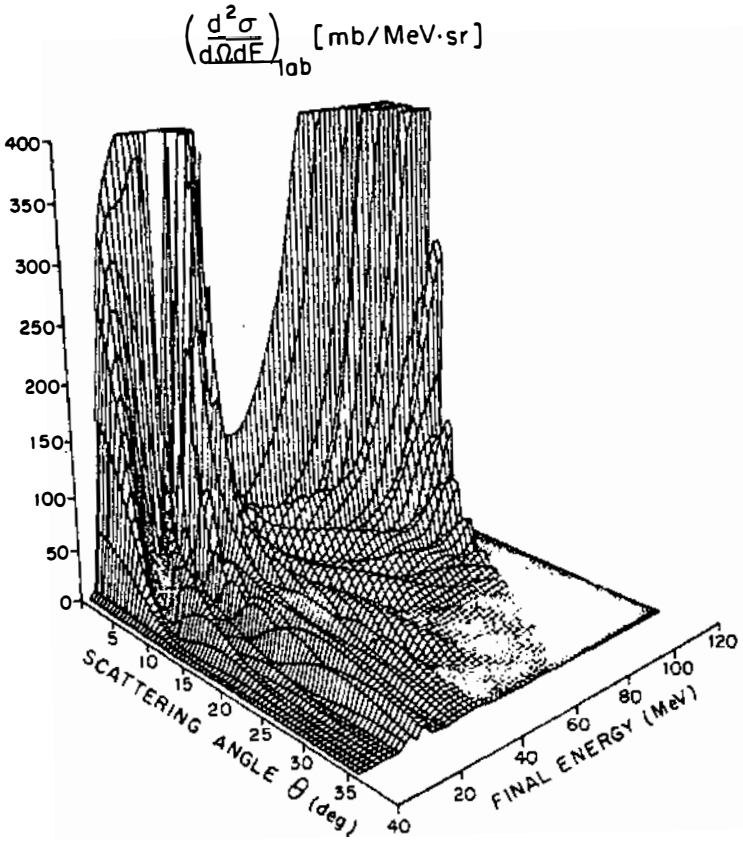


Fig. 3: The doubly differential cross section.

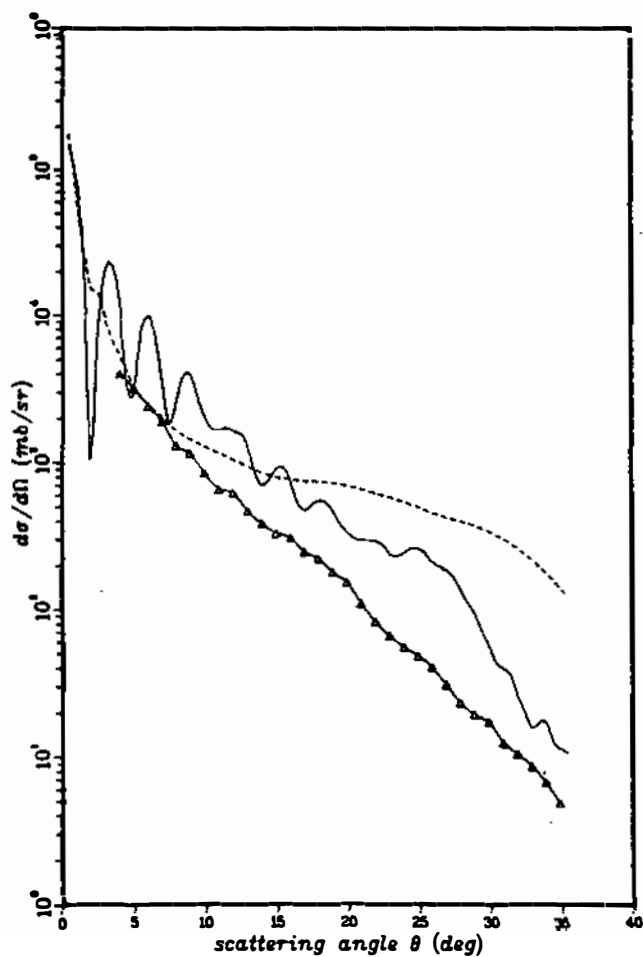


Fig. 4: Differential cross section for direct inelastic scattering integrated in energy. Solid curve - present theory, connected triangles-experiment, dashed-curve - feed-through scattering.

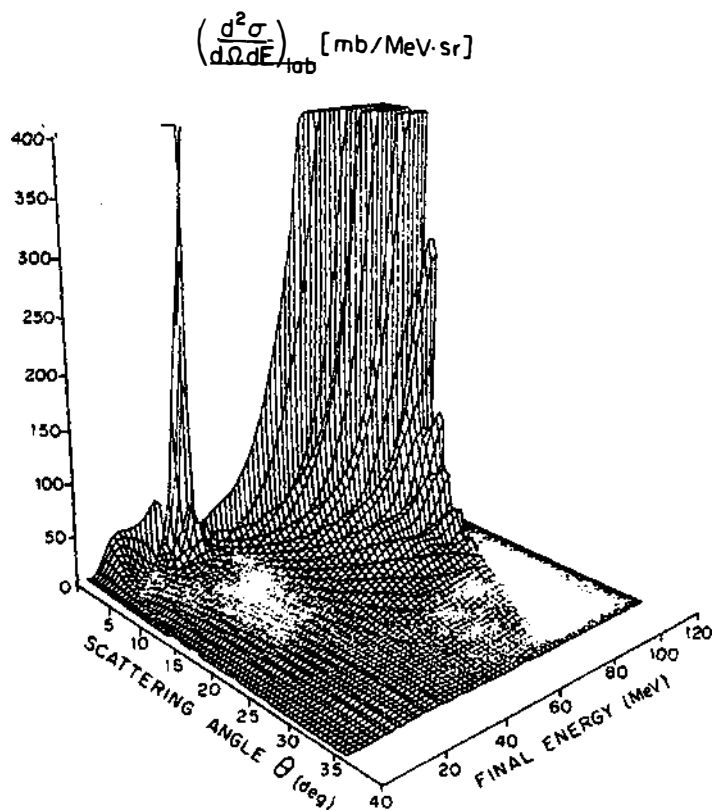


Fig. 5: Same as Fig. 3, but with "feed-through" scattering suppressed (see text).

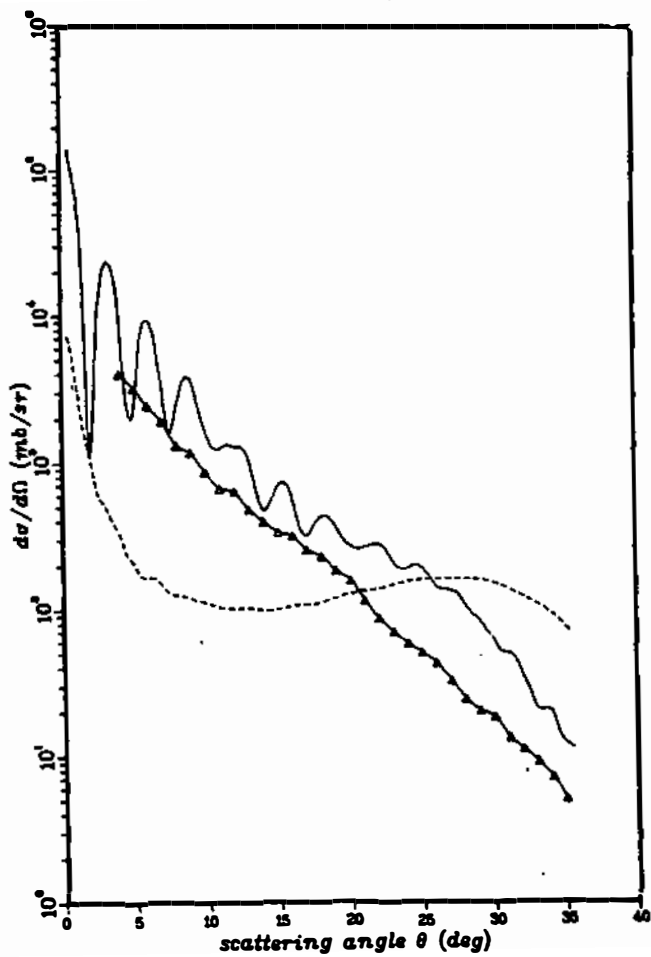


Fig. 6: Same as Fig. 4, but with "feed-through" scattering suppressed.

DISCUSSION

A. Weiguny: I am a little surprised to see that with a discretization length of 1 fm you can go up to 100 MeV in scattering energy. Resonating group calculations show that the ion - ion potential fluctuates considerably over a length of 0.5 fm.

J.A. Maruhn: The TDHF equations are very stable and tend to promote smoothness in the solutions, so that even at these energies we do not need better spatial resolution. Remember also that the nucleonic wave functions in the ground state have an internal energy that is much larger than the additional energy of translation. Numerically, of course, we have a very sensitive check - if the representation became inadequate, we would lose energy and norm very rapidly.

K. Goeke: In the adiabatic time dependent Hartree-Fock theory one is interested in a special sort of TDHF trajectories i.e. those, whose time-even part is invariant against a variation of the modulus of the initial velocity. Did you investigate your trajectories in this sense and did you perhaps find those ATDHF trajectories?

J.A. Maruhn: We did not specially investigate this problem, but it may be of interest in this connection to mention that at low energies the trajectories seemed to scale very nicely in the initial velocity, so that this may indicate the existence of such trajectories of the type you mentioned.

J. Németh: Can you calculate the cross-section for different possible processes (for example branching ratios) in your theory? One cannot calculate them in the case of the original TDHF equations.

J. A. Maruhn: Our theory does not contain anything that would make the decomposition of the final state into different masses, charges, etc. easier than in pure TDHF, aside from the special problem of fusion. If we wanted to compute, say, branching ratios into different masses we would still have to use

the pure TDHF prediction based on the final wavefunction.

R.W. Hasse: My question concerns the use of Skyrme's interaction. One knows that Skyrme always gives too large a compressibility. In your case it is two to three times larger than the commonly accepted value of $K=150-200$ MeV. Your nuclei, hence, are too stiff which may affect the results drastically. Can you comment on that?

J.A. Maruhn: We did investigate this problem by doing a few calculations with a more general force including a ρ^3 -term, which allowed us to vary the incompressibility. We could go down to about 275 MeV and the results did not change drastically. Of course the scattering angles and final energies changed somewhat, but no qualitative change in the cross-section was to be expected from these. Naturally we cannot exclude more drastic effects at very low incompressibilities but consider them unlikely.

K. Dietrich: As you have mentioned, TDHF contains an information on the mass-distribution. It also contains information on other measurable quantities like the excitation energies and the angular momenta of the outgoing fragments. The problem is just to extract this information from the Slater determinant. Consequently, your cross-section should contain a distribution of the system with respect to these final observables. The simple classical cross-section formula you showed implies the additional assumption that all fluctuations of these observables are small.

J.A. Maruhn: I agree that we should try to get more information on these additional quantities "hidden" in the TDHF final state. For the mass distribution it was shown that only very small spreads resulted but we do not know anything reliable about the other quantities. However, there is the overriding problem of whether TDHF should be expected to yield realistic information on them - it may not be worthwhile to invest the effort if the results are of little interest.

B.G. Giraud: Concerning the question of Dietrich, the difficulty is, that when $t \rightarrow +\infty$, the TDHF determinant has not a stationary expansion into channels. Therefore one should average with respect to time in order to define cross-sections. And that time average is hard to define.