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THREE-DIMENSIONAL TIME DEPENDENT HARTREE-FOCK CALCULATIONS: APPLICATION TO  
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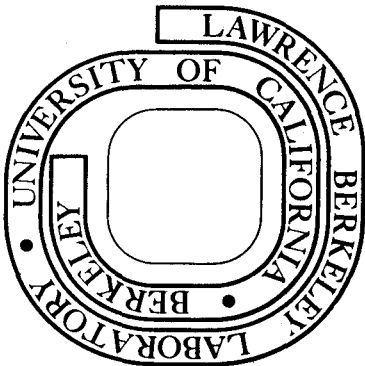
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THREE-DIMENSIONAL TIME DEPENDENT HARTREE-FOCK  
CALCULATIONS: APPLICATION TO  $^{16}\text{O} + ^{16}\text{O}$  COLLISIONS

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ABSTRACT

A coordinate-space method is developed to solve the three-dimensional time-dependent Hartree-Fock equations. It is applied to the study of  $^{16}\text{O} + ^{16}\text{O}$  collisions at  $E_{\text{lab}} = 105$  MeV for incident angular momenta from 0 to  $40\hbar$ . We find fusion for  $L = 13\hbar$  through  $27\hbar$  and highly inelastic scattering for  $L \leq 11\hbar$ .

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## I. INTRODUCTION

Time-dependent Hartree-Fock theory (TDHF)<sup>1</sup> has emerged in recent years as a promising candidate for a tractable microscopic theory of large-amplitude collective motion. Although investigations of TDHF's theoretical content date from the last decade,<sup>2,3</sup> current interest in the method is due largely to the realization that it might adequately describe heavy-ion reactions and fission.<sup>4-8</sup> The first application of TDHF to reaction phenomena was made by Bonche, Koonin and Negele,<sup>9</sup> who numerically studied the one-dimensional collisions of slabs of nuclear matter. This work was followed by the studies of Cusson and Maruhn for  $^{12}\text{C} + ^{12}\text{C}$ ,<sup>10</sup> and by those of Koonin<sup>11</sup> and Koonin et al.<sup>12</sup> for  $^{16}\text{O} + ^{16}\text{O}$  and  $^{40}\text{Ca} + ^{40}\text{Ca}$ . These calculations were two-dimensional in the sense of treating axially-symmetric three-dimensional systems. In the latter paper some effects of finite impact parameters were accounted for by a phenomenological rotating frame approximation. The axially-symmetric work has been extended to the mass-asymmetric system  $^{14}\text{N} + ^{12}\text{C}$  by Maruhn-Rezwani, et al.<sup>13</sup> Some truly two-dimensional calculations of the collisions of rods of nuclear matter which allow for axial asymmetries have been performed by Bonche et al.<sup>14</sup> Fully three-dimensional calculations were first reported by Maruhn and Cusson,<sup>15</sup> who studied some collisions of  $^{16}\text{O} + ^{16}\text{O}$  using a zero-range effective interaction, and then included the Coulomb force in a more extensive series of calculations which treated the  $^{14}\text{N} + ^{12}\text{C}$  system as well.<sup>16</sup> Detailed reviews of much of this activity have been given by Kerman<sup>17</sup> and Bonche.<sup>18</sup>

In this work we present a technique for solving the TDHF equations in three dimensions (3-D) and demonstrate its application by an extensive

study of the  $^{16}\text{O} + ^{16}\text{O}$  system at  $E_{\text{lab}} = 105$  MeV. Our study is complementary to that of Bonche et al.<sup>19</sup> who have explored many energies at a limited number of impact parameters in order to determine the fusion excitation function. We feel it is important to do these calculations in 3-D so as to eliminate the necessity of assumptions other than the TDHF approximation.

Our calculations have been motivated by several considerations. At the most practical level, the non-linear nature of the TDHF equations makes analytic study impossible and numerical calculations essential. Our understanding is still at the stage of asking questions about what the TDHF equations "do." The calculations presented here impose a minimum of constraints on the symmetry of the TDHF determinant and so begin to give answers to these questions which are free from the uncertainties due to simplified geometries. They are also stringent tests of the validity of the simpler two-dimensional calculations. At the phenomenological level, TDHF has the appeal of naturally extending the shell model to dynamical problems. As a result, phenomenological models of heavy-ion reactions such as the liquid drop model<sup>20</sup> and the one-body viscosity<sup>21</sup> can be related to the independent particle picture realized in the Hartree-Fock (HF) and TDHF approaches. There are also natural analogies between TDHF and a fluid dynamical picture.<sup>22,23</sup> Our results help to understand these connections. Finally, at a fundamental level, many aspects of TDHF remain unclear. Some results have been obtained in connection with the translational invariance,<sup>2</sup> rotational invariance,<sup>3</sup> and continuity equations<sup>8,24</sup> of the theory and both the small amplitude (RPA) and adiabatic<sup>4-7</sup> limits have been related to ordinary quantum mechanics. However, the interpretation of the results of the general theory remains vague and has been limited almost exclusively to the most naive classical picture. In particular, a precise understanding

of the relationship between the TDHF initial conditions and the Schroedinger wave-packet used in ordinary time-dependent collision theories<sup>25</sup> is still missing. Quantal and classical aspects are intertwined in a way such that it is difficult to determine the predictive powers of the theory. However, our incomplete comprehension does not mean that contact with experiment is not possible, but only that we do not know how to fully extract the information contained in our results.

The remainder of the paper is organized as follows: In Section II we review the basic TDHF equations and present the effective interaction we have used. The symmetries imposed on the TDHF determinant for computational are treated in Chapter III. Section IV presents the starting conditions and Section V contains our results. Section VI is a discussion of the results, and Section VII is our conclusion. The technical details of our calculations are contained in the Appendices. Appendix A is concerned with the numerical discretization of the TDHF energy functional and its effect on the translational invariance properties of the finite difference equations. In Appendix B, we discuss several methods for evolving the three-dimensional TDHF equations with a finite time-step. Finally, Appendix C contains a discussion of a method for solving the discrete Poisson and Helmholtz equations which is necessary for obtaining the one-body Coulomb and Yukawa potentials.

## II. THE TDHF EQUATIONS

A detailed discussion of the TDHF theory can be found in many papers. For completeness, we will only outline the derivation of the equations here.

In the TDHF approximation, the many-body wavefunction of an A-nucleon system is constrained at all time to be a single Slater determinant,  $\Psi$ . The equations covering the evolution of the associated or the normal single-particle (s.p.) wavefunctions,  $\{\psi_j, j=1, \dots, A\}$  can be derived from a variational principle which makes the "action"

$$\mathcal{G} = \int_{t_1}^{t_2} dt \langle \Psi(t) | i\hbar \frac{\partial}{\partial t} - \hat{H} | \Psi(t) \rangle \quad (1)$$

stationary with respect to the variation of these wavefunctions.<sup>6,7</sup> Here,  $\hat{H}$  is the many-body Hamiltonian operator, which in practice is taken to be the kinetic energy and a two-body effective interaction. The variation of Eq. (1) then leads to the coupled TDHF equations

$$i\hbar \frac{\partial \psi_j}{\partial t} = h(t)\psi_j \quad ; \quad j = 1, \dots, A \quad (2)$$

where  $h$  is the time-dependent hermitian one-body HF Hamiltonian. A non-linear coupling among the equations (2) arises from the functional dependence of  $h$  upon the  $\{\psi_j\}$ . As a consequence, the superposition principle does not hold for the TDHF equations. Two important properties of the TDHF equations are the conservation of the total energy

$$E = \langle \Psi(t) | \hat{H} | \Psi(t) \rangle \quad (3)$$

which follows directly from the variational formulation of the theory, and the time-independence of the inner products of the  $\{\psi_j\}$  among themselves.



The most general expressions for  $E$  and  $h$  in terms of  $\hat{H}$  can be found in references 3 - 6. We shall henceforth consider only the effective interaction used in our work and follow ref. 12 in writing the total energy as a functional of the nuclear density

$$\rho(\vec{r}) = \sum_{j=1}^A |\psi_j(\vec{r})|^2 \quad (4)$$

and the kinetic energy density

$$\tau(\vec{r}) = \sum_{j=1}^A |\nabla\psi_j(\vec{r})|^2 \quad (5)$$

$$\begin{aligned} E = & \int d\vec{r} \left[ \frac{\hbar^2}{2m} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^3 \right] \\ & + \frac{1}{2} V_0 \int d\vec{r} \int d\vec{r}' \rho(\vec{r}) \frac{e^{-|\vec{r}-\vec{r}'|/a}}{|\vec{r}-\vec{r}'|/a} \rho(\vec{r}') \\ & + \frac{1}{2} e^2 \int d\vec{r} \int d\vec{r}' \rho_p(\vec{r}) \frac{1}{|\vec{r}-\vec{r}'|} \rho_p(\vec{r}') \end{aligned} \quad (6)$$

The first term in the brackets is the kinetic energy, while the following two terms are the expectation value of the zero-range density-dependent two-body effective interaction

$$t_0 \delta(\vec{r}_1 - \vec{r}_2) + \frac{t_3}{6} \rho\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right) \delta(\vec{r}_1 - \vec{r}_2) \quad (7)$$

The last two terms in Eq. (7) are the expectation values of a Yukawa interaction and the direct Coulomb interaction ( $\rho_p$  is the proton density defined similarly to Eq. (4)).

The functional variation of the energy  $E$ , as depicted in Eq. (6), with respect to the  $\{\psi_j^*\}$  leads directly to the TDHF one-body Hamiltonian

$$h = -\frac{\hbar^2}{2m} \nabla^2 + \frac{3}{4} t_0 \rho + \frac{3}{16} t_3 \rho^2 + W_Y + W_C \quad (8a)$$

Here, the Yukawa potential is

$$W_Y(\vec{r}) = V_0 \int d\vec{r}' \frac{e^{-|\vec{r}-\vec{r}'|/a}}{|\vec{r}-\vec{r}'|/a} \rho(\vec{r}') \quad (8b)$$

and the Coulomb potential (which is effective only for protons) is

$$W_C(\vec{r}) = e^2 \int d\vec{r}' \frac{1}{|\vec{r}-\vec{r}'|} \rho_P(\vec{r}') \quad (8c)$$

Equations (2) and (8) are the TDHF equations we solve by means of the coordinate-space methods outlined in the appendices. The parameters  $t_0$ ,  $t_3$ ,  $V_0$  and  $a$  used in the present paper are those of Ref. 12 and are given below in Table 1.

TABLE 1. Values of the coefficients of the Skyrme and the Yukawa interaction.

$t_0$ MeV fm <sup>3</sup>	$t_3$ MeV fm <sup>6</sup>	$V_0$ MeV	$a$ fm
-497.66	17288	-363.044	0.4598

### III. SYMMETRIES

The history of numerical TDHF calculations has been one of the gradual relaxation of symmetry constraints imposed on the determinantal wavefunction. Such symmetries have been useful in reducing the magnitude of the numerical effort involved and have therefore allowed basic investigations of the TDHF equations. However, it now seems probable that a full test of the possibilities of the TDHF theory in realistic situations will require the breaking of as many symmetries as is possible. Unfortunately, while we would like to relax as many "built-in" constraints as we can, practical reasons have forced us to retain the four symmetries we discuss below.

In solving the TDHF equations we have assumed a perfect spin-isospin degeneracy, so that each spatial orbital is occupied by four nucleons. In this case, the proton density in Eqs. (6) and (8) is replaced by one-half of the nucleon density and the Coulomb potential (Eq. (8c)) acts on all spatial orbitals. This imposed degeneracy makes our calculations applicable only to 4-N systems. Since each spatial orbital is then effectively occupied by an  $\alpha$  particle, one or two nucleon transfer are not accurately described in our model and nucleon emission (which does occur in TDHF!<sup>7</sup>) is incorrectly accounted for. The isospin degeneracy, which is very accurately conserved in TDHF calculations of light systems which allow for the neutron-proton degrees of freedom,<sup>13,16</sup> can be easily removed with an increase of a factor of two in computing time and storage. Removal of the spin degeneracy would be more complicated. A spin-orbit interaction demands that each wavefunction be partially spin-up and spin-down. Therefore, including the spin degree of freedom would increase storage and computation by at least a factor 4.

We have also imposed two spatial symmetries on the TDHF determinant. These are reflection symmetry with respect to the reaction plane (taken to be the  $Z=0$  plane), and point reflection symmetry through the center-of-mass (c.m.) of the total system (taken to be the origin). These symmetries, together reduce our numerical effort by a factor of four. In Appendix A we show how practically they have been implemented in our calculation

Of the two spatial symmetries, the second is probably the more restrictive, since it limits the calculations to systems of two identical ions. However, it seems unlikely that mass-asymmetric degrees of freedom would be significant in an unconstrained calculation of the light symmetric systems we consider here. Despite the four symmetries we have imposed, our calculations represent a significant advance over the previous two-dimensional work.<sup>10-13</sup> As we shall see in Sections V and VI, the inclusion of triaxial degrees of freedom leads to substantial qualitative effects on the TDHF results,\* although axial symmetry appears to be an adequate approximation for nearly head-on collisions. Of course, the effects of the centrifugal force due to finite impact parameters are naturally taken into account in our 3-D calculations and we do not have to make any assumptions about the moment of inertia, as is done in Ref. 12.

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\*In terms of the usual  $\beta, \gamma$  parameterization of triaxial shapes,<sup>26</sup> the dynamics of the two-dimensional calculations are restricted to the lines  $\gamma=0$  and  $\gamma = \pi/3$ , while our three-dimensional calculations cover the entire range  $0 \leq \gamma \leq \pi/3$ .

#### IV. INITIAL CONDITIONS

The TDHF equations (2) are first-order in time, so that the values of all of the single-particle wavefunctions at some time  $t=0$  are required as initial conditions. Since we solve the equations in the overall c.m. frame, these should be chosen to represent identical nuclei approaching one another at a finite impact parameter with equal and opposite velocities  $\vec{v} = \pm \hbar \vec{k}/m$ . We have therefore constructed the initial state by multiplying each of the single-particle wavefunctions of the static HF solution of each nucleus\* by the phase  $e^{i\vec{k} \cdot \vec{r}}$ . In the absence of numerical inaccuracies, (cf. Appendix A), this determinant represents two  $^{16}\text{O}$  nuclei which translate uniformly with the required velocities prior to collision. In practice, we start the nuclei along the classical Coulomb trajectory they would have followed from infinity to the relatively large separation we choose at  $t=0$  ( $\sim 16$  fm). Our initial conditions therefore neglect the presumably small effects of Coulomb-induced deformations prior to  $t=0$ .

Such an initial condition is usually interpreted as a wave-packet despite the fact that we have only multiplied the static Slater determinant by the plane wave  $\exp(i\vec{k} \cdot \vec{R})$ , where  $\vec{R} = \sum_{j=1}^A \vec{r}_j$ . In fact the wave packet is already contained in the static HF solution which is not an eigenstate of the total momentum. If we assume that we can factor out the center-of-

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\*To find the static HF solutions used in our calculation, we evolve equations similar to (2) and (8), beginning with an arbitrary trial determinant constructed from single-particle orbitals with the required symmetries. The evolution is done on the discrete spatial mesh described in Appendix A, using an evolution method similar to those described in Appendix B with the replacement  $\Delta t \rightarrow i\Delta t$ . When the single particle wavefunctions are orthonormalized after every "time" step there is rapid convergence to the ground state solution, provided the magnitude of  $\Delta t$  is sufficiently small.

mass motion\* we may write

$$\psi_{\text{HF}}(\text{static}) = G(\vec{R})\chi \quad (9)$$

where  $G(\vec{R})$  stands for the wavefunction of the c.m. and  $\chi$  for the internal wavefunction. The Fourier transform of  $G(\vec{R})$  would be the wave-packet in momentum space. The only result achieved by the multiplication by  $e^{i\vec{k}\vec{R}}$  is a shift of the center of momentum of this wave-packet by the vector  $\vec{k}$  without any change in its shape. The translating TDHF wavefunction would then be

$$\psi_{\text{TDHF}}(\text{translating}) \approx e^{-i \frac{t}{\hbar} \left( \sum_{j=1}^A \left( \epsilon_j + \frac{\hbar^2 \vec{k}^2}{2m} \right) \right)} G(\vec{R} - \vec{v}t)\chi \quad (10)$$

In Eq. (10), the  $\epsilon_j$  are the static HF single-particle energies. For a  $^{16}\text{O}$  nucleus of oscillator wavefunctions, the kinetic energy associated with the c.m. motion is 1/24 of the total kinetic energy. Using this ratio for the static HF wavefunction we find a spread in energy of about 10 MeV. A direct correspondence of the TDHF wave packet to a Schroedinger wave-packet would lead us to conclude that 10 MeV gives a measure of the energy resolution of the incident beams associated with each  $^{16}\text{O}$  nucleus.

There are, however, several crucial differences between translating a TDHF solution and a Schroedinger wave-packet. These come mainly from the non-linearity of the TDHF equations, which is itself a consequence of the restricted variational space (one Slater determinant) used in the theory. We are not free to change arbitrarily the shape of the c.m. wave-packet. The static HF

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\*This is certainly a good approximation for an  $^{16}\text{O}$  nuclei. Indeed, the HF single-particle orbitals of light nuclei are very close to oscillator wave functions, for which the factorization is exact.

equations give at the same time the wavefunctions for the internal degrees of freedom and for the center of mass. In contrast to the Schroedinger picture, all the degrees of freedom are coupled by the minimization process in the space of the Slater determinants.\* The same coupling is responsible for the fact that the TDHF wave-packet does not spread as a function of time,<sup>†</sup> as does the Schroedinger wave-packet. In fact, formula (10) is identical to the formula (15) of Ref. 25 describing a Schroedinger wave-packet in the limit where spreading is neglected. In the same reference one finds an expression (formula 19) for a quantity  $e$  which should stay small for the spreading of the wave-packet to be negligible.

$$e = \frac{1}{w} \left( \frac{\Delta t \hbar}{2wM} \right) \quad (11)$$

Here  $\Delta t$  is the total time, during which the wave-packet is followed,  $w$  the spatial width of the function  $G(\vec{R})$ , and  $M$  the total mass of the system. If we use  $\Delta t = 10^{-21}$  s, which corresponds in our calculations to a typical full collision time, then  $e = 0.5$  (we take  $w = 2$  Fm). This number is certainly not negligible, but may be sufficiently small to allow correspondence between the TDHF solution and a Schroedinger wave-packet. If we were to adopt this viewpoint, then quantitative comparison between our results and a normal Schroedinger equation would require an understanding of the evolution of a Schroedinger wave-packet with 10 MeV spread during a collision over times of the order of  $10^{-21}$  s.

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\*One could imagine changing the shape of the HF wave-packet by solving the static equations with an external constraint like  $\vec{P}^2$  where  $\vec{P}$  is the total momentum. However, this would induce a change in the internal wave-function  $\chi$ .

<sup>†</sup>Except for the trivial case  $A = 1$ , where the HF and Schroedinger wave-packet are identical.

An alternative position one may take is that we are really only interested in following the wave-packet for  $2 \times 10^{-22}$  sec, the time for our nuclei to move from their initial position to contact. Then  $e = 0.1$  and one does not have to worry about spreading.

In the following we shall mainly interpret our TDHF results from a classical point of view. This is consistent with the fact that a non-spreading wave-packet is the characteristic of a classical particle as can be seen from the linear dependence of the spreading parameter  $e$  on  $\hbar$  (formula 11).



## V. RESULTS

Our numerical methods provide, at each time step, the set of s.p. wave-functions  $\psi_j(\vec{r}, t)$ , or equivalently, the one-body density matrix. Because this represents far more information than can be comprehended easily, we have elected to display some of the physically relevant quantities derivable from these wave-functions.

In Figs. 1-3 we show the nucleon density  $\rho$  at various times for collisions with impact parameters corresponding to  $L = 40\hbar$ ,  $L = 13\hbar$ , and  $L = 5\hbar$ . The figures show contour plots of the density integrated along the direction perpendicular to the reaction plane.

For the largest value of the angular momentum ( $L = 40\hbar$ ) the nuclei appear to pass each other without excitation. A comparison with the classical Coulomb trajectory shows that indeed no nuclear interaction takes place and that Coulomb excitation is negligible. Within the precision of our calculation,  $L = 40\hbar$  corresponds to the minimum angular momentum for pure Coulomb scattering.

For a smaller value of the angular momentum ( $L = 13\hbar$ ), the collision leads to fusion. The two nuclei remain in contact for a time longer than  $3 \times 10^{-21}$  sec; the time at which we stopped this calculation. Some shapes exhibit strong non-axial deformations. In fact, the analysis of the quadrupole moment tensor shows that the  $\gamma$  asymmetry angle sometimes reaches values higher than  $20^\circ$  (for  $L = 15\hbar$ ,  $\gamma$  has temporarily exceeded  $30^\circ$ ).

At an even smaller impact parameter ( $L = 5\hbar$ ), fusion no longer occurs and two fragments emerge directly after the collision.\* One must remember

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\*The density at the origin does not go back to exactly zero after the separation of the main fragments. It stays within  $10^{-3}$  to  $10^{-2}$  of the density in the center of the outgoing fragments (to be compared to the value  $10^{-7}$  before the collision). We cannot determine whether this is due to some small probability fusion process or to numerical inaccuracies. In the same analogous way, when a fusion takes place (as with  $L = 13\hbar$ ), the density at the edges of the box gradually rises to a  $10^{-3}$  to  $10^{-2}$  ratio to the density at the origin, as if some matter was being radiated out of the fused system.

that these fragments do not correspond to only  $^{16}\text{O}$  nuclei since some transfer has occurred during the reaction.<sup>12</sup> In addition, a large amount of the initial kinetic energy ( $\sim 80\%$ ) has been transferred to internal degrees of freedom, as can be seen in the large octupole oscillations of the fragments after the collision.

A more physical description of the collision process can be obtained by plotting the trajectories of the c.m. of each fragment for different  $L$ . However, the reduction of such a complex dynamical system to a single coordinate can lead to some unusual effects, as we discuss below. In addition, there is no unique way to define a fragment and this notion even loses meaning for complete fusion configurations. In this paper we have adopted the following definition. After having determined the principal axes of the inertia tensor of the mass density, we define a fragment as the matter located on one side of the inertial axis associated with the largest eigenvalue and then take its center of mass.\*

In Fig. 4 we have plotted the trajectories of the vector  $\vec{R}$  joining the c.m.'s of the fragments for several values of the angular momentum.

The trajectories can be divided into three groups. Large values of  $L$  ( $L > 27\hbar$ ) do not lead to fusion. As mentioned before,  $L \geq 40\hbar$  yields pure Coulomb scattering. The rainbow angular momentum is found around  $35\hbar$ , and between  $L = 30\hbar$  and  $L = 27\hbar$  the deflection angle becomes negative

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\*Another possible prescription consists in diagonalizing the mass quadrupole tensor and choose the orientation of the c.m.'s axis as those associated with the largest moment  $Q$  ( $Q > 0$ ). The distance  $R$  between the c.m.'s of the two  $^{16}\text{O}$  is then defined as  $R = (Q/A)^{1/2}$ , where  $A = 16$  in our case. For the results presented here, this definition and the one used above lead essentially to the same trajectories. The difference in the angle never exceeds  $2^\circ$  and the difference in distances  $R$  is never larger than  $0.3$  fm. A significant difference would only occur for very compact mass distributions.

as the nuclear attraction overcomes the Coulomb repulsion.

The second group of trajectories leads to fusion ( $13\hbar \leq L \leq 27\hbar$ ). Different examples of these are shown separately in Fig. 5. They are qualitatively very different. For the large values of  $L$  ( $L = 27\hbar$  and  $25\hbar$ ) the dominant factors are the nuclear attraction combined with dissipation. These lead to a smooth orbiting trajectory. For lower impact parameters ( $L = 13\hbar$  and  $20\hbar$ ) the trajectory is more complex. After an initial attraction the two nuclei reach a configuration where the collective potential leads to a repulsion. As the nuclei begin to move apart under the influence of this repulsion, they are unable to separate because of the large amount of energy that has been dissipated.

The third group of trajectories ( $L < 13\hbar$ ) does not lead to fusion. We therefore do not find the expected result that fusion, if it occurs, does so at zero impact parameter. The existence of a low  $L$  window for which fusion does not occur is energy-dependent. Indeed, we show in Fig. 6 an example of a trajectory at much lower energy ( $E_{\text{lab}} = 32$  MeV) for which a head-on collision does lead to fusion. This had already been noted in Ref. 12 for the  $^{40}\text{Ca} + ^{40}\text{Ca}$  system.

In Fig. 7 we display a collision at  $E_{\text{lab}} = 192$  MeV and a large impact parameter, 6 fm ( $L = 42\hbar$ ). This figure complements Fig. 2 which showed a fusion process for a small value of the impact parameter. Non-axial effects are very important. A comparison of the shapes at  $t = 7 \times 10^{-22}$  s and  $15 \times 10^{-22}$  s shows two extreme stages of a wiggling mode. Note how the shape becomes more compact (i.e. more fused) during the collision. A more detailed study of the fusion regime may be found in Ref. 19.

In Fig. 8 we give the deflection angle and the total kinetic energy loss (in the c.m. frame) as a function of the angular momentum. For small

impact parameters ( $L < 13\hbar$ ) the kinetic energy loss is constant at about 35 MeV to be compared to the 52.5 MeV available initially in the center-of-mass frame. Because of the total c.m. motion these trajectories would result in the fragments moving forward in the laboratory frame. According to our calculations, one would expect heavy fragments moving with kinetic energy ranging between 5 and 65 MeV in a forward cone of about  $35^\circ$ . (Recall that the beam energy is 105 MeV.) Since the fragments are strongly excited the mass distribution would certainly not be centered around  $A = 16$  due to de-excitation via nucleon or alpha particle emission. When the fragments emerge, they have nearly the same angular momentum with which they enter. This is in spite of the fact that at times during the collision the total angular momentum is almost entirely absorbed by the internal angular momentum of the fragments.

There is a difference between our results and those of Ref. 16, since we do get fusion. Because the energy used for the  $^{16}_O + ^{16}_O$  collisions in Ref. 16 is slightly higher than the one we use (8 instead of 6.6 MeV per nucleon in the lab) we have made one calculation with the energy of Ref. 16 and with an angular momentum  $L = 30\hbar$ . Consistent with our previous results we find fusion. The trajectory was followed up to a deflection of  $-3\pi/2$  without any indication of separation, in contrast to the finite deflection angle,  $-\pi/3$  found in Ref. 16 (Fig. 7). The difference could come from our inclusion of a Yukawa interaction not present in their calculation. Our interaction provides a better reproduction of the surface of the nuclei, a feature which is certainly needed to describe correctly the heavy-ion collisions. However, the apparent sensitivity to the interaction indicated by their results lead us to hope that TDHF calculations combined with appropriate experiments will

lead to increasing our knowledge of the effective interaction.<sup>19</sup>

## VI. DISCUSSION

The most striking feature of our results is the absence of fusion for small values of the incident angular momentum. We find that for any angular momentum from 13 to  $27\hbar$  the nuclei "fuse" in the sense that they remain either in close contact for times larger than  $3 \times 10^{-21}$  sec or that the deflection angle exceeds  $-180^\circ$ . If we interpret this range of impact parameters classically we obtain a fusion cross section of about 0.8 barns.

All trajectories with  $L \leq 20\hbar$  exhibit a loop at the point of closest approach, as can be seen in Figs. 4 and 5. At this point, the relative orbital angular momentum of the fragments has become negative, changing sign from its value at  $t=0$ . This phenomena has its origin in the single-particle degrees of freedom treated explicitly in a TDHF calculation. Similar behavior, which is due to the motion of the single-particle wavefunctions in the time-dependent mean field, has been observed in both one-<sup>9</sup> and two-dimensional<sup>12</sup> calculations; we shall sketch the same reasoning here to explain our three-dimensional results. When the two nuclei begin to interact, the barrier between their separate mean field potentials disappears and all wavefunctions begin to move in one large common well. The velocities of the orbitals from one nucleus as they traverse the other nucleus differ according to their internal kinetic energy. Thus, in the  $^{16}\text{O} + ^{16}\text{O}$  system, some 1p orbitals move faster and

reflect first from the opposite wall of the potential. Their resulting backward motion cancels the still forward motion of the remainder of the orbitals. As a result, the net orbital angular velocity of the fragment c.m.'s can become negative. This example of the exchange of angular momentum between single-particle and collective degrees of freedom is the essence of the one-body dissipation process. However, in this relatively small system, the non-statistical dynamics of a few orbitals soon restores much of the angular momentum to the c.m. motion. In fact, there is hardly any angular momentum loss in the low impact-parameter events. In heavier systems, the greater diversity of single-particle motions will affect the collective variables in a much smoother manner, so that the notion of a macroscopic dissipation coefficient will become applicable.<sup>19</sup> One can also note that the significant differences between the different fusion trajectories  $13\hbar \leq L \leq 27\hbar$  (Fig. 5) would be difficult to reproduce by a model taking only into account the motion of the c.m.'s.

We have shown that it is unlikely that one could explain all our results by a potential and a viscosity coefficient. However, this is possible within a limited range of angular momenta. We demonstrate this for the low values of the angular momentum which lead to inelastic scattering.

For values of  $L$  between 0 and  $20\hbar$ , the point of closest approach corresponds to an almost constant value of the distance between the c.m.'s: 4.1 fm (see Fig. 4). This gives us the location,  $R_B$ , of the internal repulsive part of the heavy-ion nuclear potential\* (Fig. 9). This internal

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\*Effective mass effects are neglected, as it can generally be done in a one-dimensional problem by a proper re-definition of the potential. The mass is therefore the reduced mass  $\mu = 8m$ .

barrier is of dynamical origin, and probably comes from the inability of the fragments to significantly change their shell structure during the collision. Static constrained HF calculations performed for the same system,<sup>27</sup> which can be thought of as describing the potential for an infinitely slow collision, do not give a potential with an internal barrier. There, the system of 32 nucleons adjusts itself to the best possible shell structure for a given separation of the c.m.'s. For small separations, the  $^{32}\text{S}$  configuration is energetically the most stable. Figure 10 shows the behavior of the s.p. energies as a function of time for a nearly head-on collision ( $L = 0.5\hbar$ ,  $E_{\text{lab}} = 105 \text{ MeV}$ ). Initially, this s.p. spectrum exhibits the degeneracy characteristic of two  $^{16}\text{O}$  nuclei.<sup>†</sup> The degeneracy is lifted during the collision, although the shell structure is remarkably well preserved and the spectrum never comes close to that of  $^{32}\text{S}$ . Since the distance of closest approach,  $R_B$ , is almost independent of the angular momentum, the potential at that point must be very steep. Indeed, although the classical centrifugal energy  $\hbar^2 L^2 / 2\mu R_B^2$  changes by about 60 MeV for  $L$  varying between 0 and  $20\hbar$ , its effect on  $R_B$  is very small. This stiffness of the potential is confirmed by the fact that  $R_B$  is independent of the incident energy, as can be seen in Fig. 6 ( $E_{\text{lab}} = 32 \text{ MeV}$ ).

To pursue the analysis, the velocities of the c.m.'s must be considered. We do this in Fig. 11, which again corresponds to the  $L = 0.5\hbar$ ,  $E_{\text{lab}} = 105 \text{ MeV}$  collision. The energy  $E_C$  in the upper part of the figure is

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\*We defined the s.p. energies as the diagonal elements of the matrix  $\epsilon_{ij}(t) = \int dr \psi_i(t) \mathcal{H} \psi_j$ . It is not an unambiguous definition since the  $\psi_i$ 's are defined up to a unitary transformation. Another possibility would be to choose as s.p. energies the eigenvalues of the  $\{\epsilon_{ij}\}$  matrix. This choice would probably not change the qualitative aspect of our argument.

<sup>†</sup>Recall that our calculation does not include a spin-orbit force.

is the point Coulomb energy  $Z^2 e^2 / R$ . We have also plotted the quantity  $E_M$  which is larger than  $E_C$  by the total kinetic energy of the relative motion of the c.m.'s. The evolution of  $E_M$  can be understood in terms of a motion with dissipation in a collective potential well such as that shown in Fig. 9. Between the initial time and point A,  $E_M$  is constant.\* The point A corresponds to the beginning of the nuclear interaction; neglecting internal degrees of freedom makes  $E_M$  the total energy before the nuclear interaction begins. We have, therefore, an estimate of the distance at which nuclear effects become important:  $R_I = 8.5$  fm. Between A and B,  $E_M$  increases, corresponding to motion in the descending part of the potential. However, the increase of  $E_M$  is less than the depth of the potential  $V_M$  because of dissipation effects. For the same reason the distance between the c.m.'s at point B is larger than  $R_M$  (Fig. 9). Between B and C the potential rises, therefore  $E_M$  decreases until it equals the Coulomb energy  $E_C$ . The distance between the c.m.'s at point C gives the radius of the internal core  $R_B$ . The points D and E are the analogs of B and A on the outgoing part of the trajectory. This time, because of the dissipation effects, the distance between the c.m.'s at point D gives a lower limit for the value of  $R_M$ . The distance at the last point of interaction E is larger than the distance at point A reflecting both fragment elongation and an overall increase in the size of the fragments after the collision. For example, the root mean square radius of the fragments increases by about 0.3 fm as a consequence of

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\*The small decrease of  $\sim 1$  MeV is due to the numerical inaccuracies discussed in Appendix A. It is a measure of the precision of our calculations.



of the transfer of energy to the internal degrees of freedom of the fragments. If there were no dissipation, all the curves shown in Fig. 11 would be symmetric with respect to the vertical line going through point C. Analyzing the extrema of the energy curve  $E_M(t)$  and the distance curve  $R(t)$  with the above interpretation gives a minimum of the nuclear potential between -14 and -24 MeV at a distance between 5.5 and 6.5 fm. The upper boundary for the depth of potential (24 MeV) is obtained with the assumption that the dissipation of  $E_M$  occurs only when the two nuclei move toward each other (faster velocities). If one were to assume that the same amount of energy is lost during the ingoing and outgoing phases of motion, the lower value (14 MeV) would be obtained.

The energy loss for  $L = 0.5\hbar$ ,  $E_{lab} = 105$  MeV is about 35 MeV. Within the precision of our calculation (1 MeV) this number is constant for  $L$  varying between 0 and  $1\hbar$  (Fig. 8). This indicates that for these values of the angular momentum it is not necessary to introduce a tangential friction. Using a simple model, neglecting potential effects in first approximation and assuming a viscosity proportional to the relative radial velocity of the c.m.'s to take place for a distance equal to  $2(R_I - R_B)$ , we find that a radial viscosity coefficient of  $2 \times 10^{-22}$  MeV.fm.<sup>-2</sup> sec explains our 35 MeV energy loss. Within the same crude model this viscosity leads to a value of 0.9 MeV per nucleon in the c.m. ( $E_{lab} = 58$  MeV), for the threshold of *no fusion* at  $L = 0\hbar$ , in good agreement with the results of Ref. 19. Although we are not in a position to discuss the energy dependence of the collective potential, we note that this dependence will arise naturally in similar analysis of TDHF calculations at other energies.

## VII. CONCLUSION

The most interesting phenomenon we have observed in our calculation is a region of fusion which yields a fusion cross-section consistent with experiment.<sup>28</sup> This is in contrast to previous calculations in two dimensions<sup>11-13</sup> which showed no fusion for high-energy collisions. Therefore, triaxiality is important in the dissipative process that leads to fusion.

It is also important to note the lack of fusion for small angular momentum at high bombarding energy. For these small values of the angular momentum we calculate the scattering angle and energy loss of the outgoing fragments. These predictions are amenable to experimental verification. We also find that the absence of fusion for head-on collisions disappears at sufficiently low bombarding energies. However, our calculations contain several technical restrictions (e.g. spin, isospin, and two spatial symmetries) which may affect the specific numerical values presented in this paper.

A comparison with other 3-D calculations<sup>16</sup> indicates a dependence of the results on the effective interaction. This dependence is confirmed by the detailed study of the fusion excitation function contained in Ref. 19. For this reason the TDHF method appears as a promising tool for extracting from the experimental data on heavy-ion scattering, additional knowledge of the nucleon-nucleon effective interaction.

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## APPENDIX A: DISCRETE REPRESENTATION OF THE TDHF EQUATIONS

We solve the TDHF equations in coordinate space using methods similar to those of Refs. 9 and 12. In our three-dimensional calculations, the single-particle wavefunctions are described by their values on a uniformly spaced cartesian mesh contained within a rectangular box. Vanishing boundary conditions are imposed outside of this box. The choices of box dimensions and mesh spacing are influenced by two competing considerations. On the one hand, computing speed and storage consideration favor a small box and large mesh spacing to reduce the number of variables describing the system. On the other hand, the box must be large enough to contain the TDHF solution without the system "hitting the walls" and the mesh spacing must be small enough to give an accurate representation of the TDHF energy functional. Our method therefore employs a relatively large mesh spacing (1 fm in all three directions) yet uses high-order discretizations of the kinetic energy and Yukawa potentials. The box size has been varied according to the collision being calculated. We choose the center of the box to the time-independent c.m. of the whole system and orient the reaction plane normal to one edge (z axis). Typical box dimensions are 30 fm  $\times$  28 fm  $\times$  16 fm in the x, y, and z directions, respectively. The spatial symmetries we impose on the determinant (of Section III) restrict the actual numerical work to one-quarter of the box volume. How these symmetries are implemented in our code is described in Fig. 13. As discussed in Appendix C, the non-conservation of energy associated with the boundary conditions of the Yukawa potential provides a stringent check against spurious effects of the mesh boundaries.

A discrete representation of the TDHF Hamiltonian can be obtained by the variation of a discrete approximation to the energy functional with respect to the values of the single-particle wavefunctions at the mesh points. This procedure preserves the variational aspects of the discrete TDHF equations. It has been discussed in detail for cylindrical coordinate systems in refs. 11 and 12 and can be directly extended to three cartesian dimensions. We therefore discuss only those new problems presented by the three-dimensional calculations.

Experience has shown that the zero-range ( $t_0$  and  $t_3$ ) terms of the energy functional (Eq. (6)) are accurately discretized on our large mesh spacing by a trapezoidal approximation to the integrals (cf. Table III). Similarly, an adequate accuracy is easily achieved for the Coulomb energy (cf. Appendix C). However, the accuracy of the discrete approximations to the kinetic energy and short-range Yukawa potential is very sensitive to the mesh spacing and techniques used. We treat the kinetic energy below and discuss the Yukawa potential in Appendix C.

The total kinetic energy is the sum of the kinetic energies for each of the single-particle wavefunctions in each of the three spatial directions. It is therefore sufficient to consider a single wavefunction in one dimension. The fundamental quantity we are interested in approximating is then

$$T_i \equiv \frac{1}{2} \int_{x_i - \Delta x}^{x_i + \Delta x} dx \left| \frac{\partial \psi}{\partial x} \right|^2 \quad (\text{A.1})$$

where  $x_i$  is the coordinate at the  $i^{\text{th}}$  mesh point,  $\Delta x$  is the mesh spacing, and  $\psi(x)$  is the wavefunction. A Taylor expansion of  $T_i$  in  $\Delta x$  leads to

$$\begin{aligned}
T_i = & \Delta x |\psi_i^{(1)}|^2 + \frac{(\Delta x)^3}{3} \operatorname{Re}(\psi_i^{(1)*} \psi_i^{(3)} + |\psi_i^{(2)}|^2) \\
& + \frac{(\Delta x)^5}{60} \operatorname{Re}(\psi_i^{(1)*} \psi_i^{(5)} + 2\psi_i^{(2)*} \psi_i^{(4)} + 3|\psi_i^{(3)}|^2) + \theta((\Delta x)^7)
\end{aligned}
\tag{A.2}$$

The notation  $\psi_i^{(n)}$  is used here for the  $n^{\text{th}}$  derivative of  $\psi$  at  $x_i$ .

The lowest order difference approximation to  $|\psi_i^{(1)}|^2$  results in the three-point approximation to the kinetic energy<sup>29</sup>

$$T_i^{(3)} = \frac{1}{2\Delta x} \left( |\psi_{i+1} - \psi_i|^2 + |\psi_i - \psi_{i-1}|^2 \right) \tag{A.3}$$

The variation of the quantity  $T_i^{(3)}$  with respect to  $\psi_i^*$  leads directly to the three-point approximation for  $\psi_i^{(2)}$  used in Ref. 12. A simple analysis of  $T_i^{(3)}$  gives

$$T_i^{(3)} = \Delta x |\psi_i^{(1)}|^2 + \frac{(\Delta x)^3}{3} \operatorname{Re} \left( \psi_i^{(1)*} \psi_i^{(3)} + \frac{3}{4} |\psi_i^{(2)}|^2 \right) + \theta((\Delta x)^5) \tag{A.4}$$

so that the error term in  $T_i^{(3)}$  is  $\theta((\Delta x)^3)$ .

The next order approximation to the kinetic energy is obtained by using an approximation of the form

$$T_i^{(5)} = \frac{1}{2(\Delta x)} \left( |b_- \psi_{i-1} + b_0 \psi_i + b_+ \psi_{i+1}|^2 + |b_+ \psi_{i-1} + b_0 \psi_i + b_- \psi_{i+1}|^2 \right) \tag{A.5}$$

where the coefficients  $b_{0,\pm}$  are chosen\* so that  $T_i^{(5)}$  approximates  $T_i$

\*Our choice (A.6) is one member of a one-parameter family of complex solutions  $b_0 = 2/\sqrt{3}$ ,  $b_{\pm} = -1/\sqrt{3} \pm \frac{1}{2} e^{i\alpha}$ ,  $0 \leq \alpha \leq \pi$ . Equation (A.7) holds for any value of  $\alpha$ .

through  $\theta((\Delta x)^5)$ :

$$b_0 = \frac{2}{\sqrt{3}} \quad (\text{A.6})$$

$$b_{\pm} = -\frac{1}{\sqrt{3}} \pm \frac{1}{2}$$

The variation of  $T_j^{(5)}$  leads to a five-point approximation to  $\psi_i^{(2)}$ .<sup>29</sup> The error term is  $(\theta(\Delta x)^5)$ .

$$T_i - T_i^{(5)} = \frac{(\Delta x)^5}{90} \operatorname{Re} \left( \psi_i^{(2)*} \psi_i^{(4)} + 2|\psi_i^{(3)}|^2 \right) \quad (\text{A.7})$$

The use of the five-point approximation for the kinetic energy operator complicates the time-evolution of the TDHF equations. For example, in one dimension the HF Hamiltonian is then represented by a penta-diagonal matrix, rather than a tri-diagonal one. However, in view of the 1 fm mesh spacing we are forced to use, the extra effort is justified, as can be seen by a simple example. We have calculated the kinetic energy of the lowest state in a one-dimensional oscillator potential with oscillator parameter  $m\omega/\hbar = 0.275 \text{ fm}^{-2}$ , a typical number for the nucleon problems. The results of the three- and five-point formulae with various mesh sizes are shown in Table II. The superiority of the five-point method is evident. In fact, with a mesh spacing of 1 fm, this method is more accurate than the three-point method with  $\Delta x = 0.5 \text{ fm}$ .

The translational invariance of the TDHF equations is also affected by our discretization procedure. We apply the gauge transformation  $e^{i\vec{k}\cdot\vec{r}}$  to the orbitals of the static HF solution in order to generate the initial state of a nucleus moving with velocity  $\vec{v} = \hbar\vec{k}/m$ . Because we use a Gallilean-invariant two-body interaction, the HF potential is unaffected

by this boost and the single-particle kinetic energy of each orbital increases by the translational kinetic energy  $E_T = \frac{1}{2}mv^2$ . Although these properties are true for the TDHF equations, they need not hold for their discrete approximations. In order to test this aspect of our discretization, we have applied various boosts to the ground-state oscillator wavefunction used to construct Table II. Our results are shown in Fig. 13 where we display the fractional difference between the calculated kinetic energies of the boosted and stationary states. For the calculations presented in this paper ( $E_T \leq 2$  MeV), the general level of accuracy should be 1 to 2% and for  $E_T < 25$  MeV, the five-point formula with  $\Delta x = 1$  fm is more accurate than the three-point formula with  $\Delta x = 0.5$  fm. However, some caution is necessary in applying these results to our actual calculations. Figure 13 refers to the lowest state of an oscillator well. However, our nuclei also contain p-shell orbitals. The difference formulae are less accurate for these higher lying states, so that for  $^{16}\text{O}$ , the translational kinetic energy of the boosted nucleus is in error by as much as 5%. The different errors in the different wavefunctions also lead in a different way to the breaking of translational invariance for the discrete equation. Because of differencing errors, the transformation  $e^{i\vec{k}\cdot\vec{r}}$  sets each orbital in motion with a slightly different velocity. Since the HF mean field binds all orbitals together, some energy is gradually transferred from translation into internal excitation. In  $^{16}\text{O} + ^{16}\text{O}$ , this phenomenon leads to at most a 7% loss in translational kinetic energy in our calculation over a time of  $1.5 \times 10^{-21}$  sec.

We close this appendix with an overall assessment of the accuracy of our discretization of the energy functional. We consider two  $^{16}\text{O}$



nuclei built from oscillator wavefunctions ( $m\omega/\hbar = 0.275 \text{ fm}^{-2}$ ) and positioned 16 fm apart. They are boosted toward each other with a translational kinetic energy per nucleon of  $E_T = 1.74 \text{ MeV}$ . In Table II we show the calculated ( $\Delta x = \Delta y = \Delta z = 1 \text{ fm}$ , five-point formula) and analytic contributions to the energy functional. The Coulomb and Yukawa energies have been calculated as described in Appendix C; the overall accuracy is quite acceptable, with the most serious discrepancy being some 3 MeV out of 460 MeV in the kinetic energy.

TABLE III. Contributions to the total energy of two  $^{16}\text{O}$  nuclei, as described in the text (values in MeV).

	Kinetic energy	Contribution of $t_0 \delta(\vec{r}_1 - \vec{r}_2)$	Contribution of $t_3/6 \rho \delta(\vec{r}_1 - \vec{r}_2)$	Yukawa energy	Coulomb energy
Discrete energy functional	457.560	-423.785	230.088	-458.594	36.752
Analytic value	460.504	-423.784	230.100	-458.393	36.489

TABLE II. The kinetic energy of the ground-state of a one-dimensional oscillator potential ( $m\omega/\hbar = 0.275 \text{ fm}^{-2}$ ) calculated with the three- and five-point formulae.  $\Delta x$  is the mesh spacing.

$\Delta x$ (fm)	Kinetic energy (MeV)	3-point formula	5-point formula
Analytic value		2.8512	
0.5		2.8269	2.8507
0.75		2.7968	2.8485
1.0		2.7554	2.8430
1.25		2.7034	2.8320

## APPENDIX B: SOLUTION OF THE TDHF EQUATIONS WITH A FINITE TIME STEP

I. Conservation of the Total Energy

Although the discussion contained in this paragraph is valid for any two-body interaction, we discuss here only the case of a zero-range interaction which depends linearly on the density. We therefore deal only with the density and the kinetic energy density (formulae 4, 5). However, it is straightforward to show that our arguments can be extended to the full one-body density operator, i.e., to any two-body interaction. We shall also neglect the spin and isospin degrees of freedom which are irrelevant to the argument.

If  $\{\psi_j^{(n)}\}$  ( $1 \leq j \leq A$ ) is a set of single-particle wavefunctions at time step  $n$ , the HF energy at that time step for a two-body interaction  $v_2$

$$v_2 \equiv t_0 \delta(\vec{r}_1 - \vec{r}_2) + \frac{t_3}{6} \rho\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right) \delta(\vec{r}_1 - \vec{r}_2)$$

is

$$E^{(n)} = \int d\vec{r} \left( \frac{\hbar^2}{2m} \tau^{(n)}(\vec{r}) + \frac{3}{8} t_0 \rho^{(n)}(\vec{r})^2 + \frac{1}{16} t_3 \rho^{(n)}(\vec{r})^3 \right) \quad (\text{B.1})$$

where  $\rho^{(n)}(\vec{r})$  and  $\tau^{(n)}(\vec{r})$  are, respectively, the density and kinetic energy density at time-step  $n$ .

If  $\{\psi_j^{(n+1)}\}$  is the set of single-particle wave-functions at time-step  $(n+1)$ , we define the quantity  $\delta\rho$  as

$$\delta\rho \equiv \rho^{(n+1)} - \rho^{(n)} = \sum_{j=1}^A |\psi_j^{(n+1)}|^2 - |\psi_j^{(n)}|^2 \quad (\text{B.2})$$

In the same way we have

$$\delta\tau \equiv \tau^{(n+1)} - \tau^{(n)} \quad (\text{B.3})$$

Some algebraic manipulations then show that

$$\rho^{(n+1)2} = \rho^{(n)2} + \delta\rho(\rho^{(n+1)} + \rho^{(n)}) \quad (\text{B.4})$$

$$\rho^{(n+1)3} = \rho^{(n)3} + \delta\rho(\rho^{(n+1)2} + \rho^{(n)}\rho^{(n+1)} + \rho^{(n)2}) \quad (\text{B.5})$$

These equations are exact and do not represent a truncated expansion of  $\rho^{(n+1)2}$  and  $\rho^{(n+1)3}$ . With Eqs. (B.4 and B.5) the energy at time  $n+1$ ,  $E^{(n+1)}$  can therefore be written as

$$E^{(n+1)} = E^{(n)} + \sum_{j=1}^A \int d\vec{r} \left( \psi_j^{(n+1)*} h^{(n+\frac{1}{2})} \psi_j^{(n+1)} - \psi_j^{(n)*} h^{(n+\frac{1}{2})} \psi_j^{(n)} \right) \quad (\text{B.6})$$

where the Hamiltonian  $h^{(n+1)}$  is defined as

$$h^{(n+1)} = -\frac{\hbar^2}{2m} \Delta + \frac{3}{8} t_0 \left( \rho^{(n)} + \rho^{(n+1)} \right) + \frac{1}{16} t_3 \left( \rho^{(n)2} + \rho^{(n)}\rho^{(n+1)} + \rho^{(n+1)2} \right)$$

In order to conserve the energy exactly, the  $\psi_j^{(n+1)}$ 's must be constructed so as to cancel the second term of the right-hand side of (B.6). Then choosing

$$\psi_j^{(n+1)} = U \psi_j^{(n)} \quad (\text{B.7})$$

where  $U$  is *any* unitary operator which commutes with  $h^{(n+\frac{1}{2})}$  will lead to an exact cancellation of  $(E^{(n+1)} - E^{(n)})$ . Since we want, in addition to use, a numerical scheme approximating the continuous TDHF equations

$$\begin{cases} i\hbar \frac{\partial \psi_j}{\partial t} = h \psi_j \\ h = -\frac{\hbar^2}{2m} \Delta + \frac{3}{4} t_0 \rho + \frac{3}{16} t_3 \rho^2 \end{cases} \quad (\text{B.8})$$

we can use the unitary operator

$$U_E = \exp\left(-i \frac{\Delta t}{\hbar} h^{(n+\frac{1}{2})}\right), \quad (\text{B.10})$$

or any unitary approximation to the exponential, such as the Crank-Nicholson (CN) operator:

$$U_{\text{CN}} = \frac{1 - \frac{i\Delta t}{2\hbar} h^{(n+\frac{1}{2})}}{1 + \frac{i\Delta t}{2\hbar} h^{(n+\frac{1}{2})}}. \quad (\text{B.11})$$

For the calculations presented in this paper we have expanded the exponential operator  $U_E$  in a power series through  $\theta(\Delta t^5)$ . Indeed, as the discretized operator  $h^{(n+\frac{1}{2})}$  amounts to a  $3000 \times 3000$  dense matrix for a typical mesh size, it would be difficult to use the exact exponential operator. In fact with a time step of  $4 \times 10^{-24}$  s, five terms in the exponential suffice to conserve the wavefunction norm to one part in  $10^6$  and the total energy of the system to better than 0.5% ( $\sim 1$  MeV) over periods longer than  $1.5 \times 10^{-21}$  s, a typical collision time.

The relation between  $h^{(n+\frac{1}{2})}$ , and the Hamiltonians  $h^{(n)}$  and  $h^{(n+1)}$  defined by

$$h^{(n)} = -\frac{\hbar^2}{2m} \Delta + \frac{3}{4} t_0 \rho^{(n)} + \frac{3}{16} t_3 \rho^{(n)2} \quad (\text{B.12})$$

is

$$h^{(n+\frac{1}{2})} = \frac{1}{2} \left( h^{(n)} + h^{(n+1)} \right) - \frac{t_3}{32} \left( \rho^{(n+1)} - \rho^{(n)} \right)^2 \quad (\text{B.13})$$

Thus the construction of  $h^{(n+\frac{1}{2})}$  requires the knowledge of the  $\{\psi_j^{(n+1)}\}$  which are not known ahead of time. In practice we use the following procedure. From the Hamiltonians  $h^{(n)}$ ,  $h^{(n-1)}$ , and  $h^{(n-2)}$ , we construct with Lagrange extrapolation a first guess of  $h^{(n+\frac{1}{2})}$ . We then compute a

a first estimate of  $\{\psi_j^{(n+1)}\}$  with  $U_E$ . We can then obtain  $h^{(n+1)}$  and a better approximation of  $h^{(n+\frac{1}{2})}$  using the formulae (B.12) and (B.13). Finally we compute the  $\psi_j^{(n+1)}$ 's with  $U_E$ . It can be shown that further iterations of this procedure combined with an exact handling of the operators  $U_E$  or  $U_{CN}$  would lead to a convergence toward the exact solution  $h^{(n+\frac{1}{2})}$ , and therefore an exact conservation of the energy. The method used in this paper has therefore the advantage of being easily controlled for any value of the time step by increasing either the number of terms in the expansion of  $U_E$  or the number of iterations in the calculation of  $h^{(n+\frac{1}{2})}$ . In practice we found that to reach a precision of 1 MeV in the conservation of the energy, one iteration in the calculation of  $h^{(n+\frac{1}{2})}$  sufficed ( $\Delta t = 4 \times 10^{-24}$  s). In addition, the precision required (i.e., the number of terms in the expansion of  $U_E$ ) to obtain the first estimate of  $\{\psi_j^{(n+1)}\}$  is less than the precision needed for the final set of  $\psi_j^{(n+1)}$ 's. In practice, the first two terms in the exponential operator are sufficient.

## II. Comparison with the Exact Solution

We will restrict our discussion to the case of the exponential operator  $U_E$  (formula (B.10)) and mention at the end of this appendix the results obtained with the CN method and two approximations of the CN method: the alternate direction (AD) and the local one-dimensional method (LOD).<sup>30</sup>

With the exponential operator the wavefunctions at time  $\Delta t$   $\{\psi_j^{(1)}\}$  are obtained from the wavefunctions at time zero  $\{\psi_j^{(0)}\}$  as

$$\psi_j^{(1)} = \exp\left(-\frac{i}{\hbar} \Delta t h^{(\frac{1}{2})}\right) \psi_j^{(0)} \quad (\text{B.14})$$

where the operator  $h^{(\frac{1}{2})}$  is constructed according to formula (B.13).

It will make the discussion shorter to restrict ourselves to the case where only two-body interactions are included in the Hamiltonian  $\hat{H}$ . The reader may convince himself that the results presented hereafter remain true when the zero-range density-dependent interaction is also present. For a Hamiltonian with only two-body interactions the operator  $h^{(\frac{1}{2})}$  may be written as

$$h^{(\frac{1}{2})} = \frac{1}{2} (h^{(0)} + h^{(1)}) \quad (\text{B.15})$$

For our purposes, it is convenient to emphasize the functional dependence of the HF Hamiltonian  $h^{(0)}$  and  $h^{(1)}$  on the wave-functions  $\psi_j$  and their conjugate  $\psi_j^*$ † by writing

$$h^{(0)} \equiv h\left(\{\psi_j^{(0)}, \psi_j^{(0)*}\}\right) \quad h^{(1)} \equiv h\left(\{\psi_j^{(1)}, \psi_j^{(1)*}\}\right) \quad (\text{B.16})$$

$$1 \leq j \leq A$$

In order to determine the precision of the exponential scheme, we shall study the derivatives

$$\left. \frac{\partial^n \psi_j^{(1)}}{\partial (\Delta t)^n} \right|_{\Delta t = 0} \quad (\text{B.17})$$

and compare them with the derivatives of the exact solution  $\psi_j(t)$

$$\left. \frac{\partial^n \psi_j}{\partial t^n} \right|_{t=0} \quad (\text{B.18})$$

---

† In this paper the functional dependence comes only through the density  $\rho$  (formula (4)) but with other interactions, such as the full Skyrme force<sup>8</sup> the kinetic energy and the current would also appear in the expression of  $h$ .

of the TDHF equations

$$\begin{cases} \frac{\partial \psi_j}{\partial t} = -\frac{i}{\hbar} h \psi_j \\ \psi_j(t=0) \equiv \psi_j^{(0)} \end{cases} \quad (\text{B.19})$$

The expression for the first three derivatives of the exact solution at  $t=0$  are

$$\left. \frac{\partial \psi_j}{\partial t} \right|_{t=0} = -\frac{i}{\hbar} h^{(0)} \psi_j^{(0)} \quad (\text{a})$$

$$\left. \frac{\partial^2 \psi_j}{\partial t^2} \right|_{t=0} = \left(-\frac{i}{\hbar} h^{(0)}\right)^2 \psi_j^{(0)} - \frac{i}{\hbar} \frac{\partial h^{(0)}}{\partial t} \psi_j^{(0)} \quad (\text{b}) \quad (\text{B.20})$$

$$\begin{aligned} \left. \frac{\partial^3 \psi_j}{\partial t^3} \right|_{t=0} &= \left(-\frac{i}{\hbar} h^{(0)}\right)^3 \psi_j^{(0)} + \left(-\frac{i}{\hbar}\right)^2 \left( h^{(0)} \frac{\partial h^{(0)}}{\partial t} + 2 \frac{\partial h^{(0)}}{\partial t} h^{(0)} \right) \psi_j^{(0)} \\ &\quad - \frac{i}{\hbar} \frac{\partial^2 h^{(0)}}{\partial t^2} \psi_j^{(0)} \quad (\text{c}) \end{aligned}$$

In the equations (B.20,a-c), the expression  $\partial h^{(0)}/\partial t$  should be understood as the one-body operator

$$\frac{\partial h^{(0)}}{\partial t} \equiv \left( \sum_{j=1}^A \frac{\partial h}{\partial \psi_j} \frac{\partial \psi_j}{\partial t} + \frac{\partial h}{\partial \psi_j^*} \frac{\partial \psi_j^*}{\partial t} \right) \Bigg|_{t=0} \quad (\text{B.21})$$

From the definition (B.14) and using (B.15), we have

$$\left. \frac{\partial \psi_j^{(1)}}{\partial \Delta t} \right|_{\Delta t=0} = -\frac{i}{\hbar} h^{(0)} \psi_j^{(0)} = \left. \frac{\partial \psi_j}{\partial t} \right|_{t=0} \quad (\text{B.22})$$



and

$$\left. \frac{\partial^2 \psi_j^{(1)}}{\partial (\Delta t)^2} \right|_{\Delta t=0} = \left( -\frac{i}{\hbar} h^{(0)} \right)^2 \psi_j^{(0)} - 2 \frac{i}{\hbar} \left. \frac{\partial h^{(1/2)}}{\partial \Delta t} \right|_{\Delta t=0} \psi_j^{(0)} \quad (\text{B.23})$$

From relation (B.15) one has

$$\begin{aligned} \left. \frac{\partial h^{(1/2)}}{\partial \Delta t} \right|_{\Delta t=0} &= \frac{1}{2} \left. \frac{\partial h^{(1)}}{\partial \Delta t} \right|_{\Delta t=0} = \frac{1}{2} \sum_{j=1}^A \left( \frac{\partial h}{\partial \psi_j} \frac{\partial \psi_j^{(1)}}{\partial \Delta t} + \frac{\partial h}{\partial \psi_j^*} \frac{\partial \psi_j^{(1)*}}{\partial \Delta t} \right) \Big|_{\Delta t=0} \\ &= \frac{1}{2} \sum_{j=1}^A \left( \frac{\partial h}{\partial \psi_j} \frac{\partial \psi_j}{\partial t} + \frac{\partial h}{\partial \psi_j^*} \frac{\partial \psi_j^*}{\partial t} \right) \Big|_{t=0} = \frac{1}{2} \left. \frac{\partial h^{(0)}}{\partial t} \right|_{t=0} \end{aligned} \quad (\text{B.24})$$

In order to obtain the last equalities in the above formula we have used the result (B.22). Finally, combining (B.23) and (B.24), we get

$$\left. \frac{\partial^2 \psi_j^{(1)}}{\partial (\Delta t)^2} \right|_{\Delta t=0} = \left. \frac{\partial^2 \psi_j}{\partial t^2} \right|_{t=0} \quad (\text{B.25})$$

A similar derivation gives for the third order derivative

$$\begin{aligned} \left. \frac{\partial^3 \psi_j^{(1)}}{\partial (\Delta t)^3} \right|_{\Delta t=0} &= \left( -\frac{i}{\hbar} h^{(0)} \right)^3 \psi_j^{(0)} + 3 \left( -\frac{i}{\hbar} \right)^2 \left. \frac{\partial}{\partial \Delta t} \left( h^{(1/2)} \right)^2 \right|_{\Delta t=0} \psi_j^{(0)} \\ &\quad - 3 \frac{i}{\hbar} \left( \left. \frac{\partial^2 h^{(1/2)}}{\partial (\Delta t)^2} \right|_{\Delta t=0} \right) \psi_j^{(0)} \end{aligned} \quad (\text{B.26})$$

Using the formulae (B.24) and (B.26) and a relation similar to (B.24) for the second derivative of  $h^{(1/2)}$ , one obtains

$$\left. \frac{\partial^3 \psi_j^{(1)}}{\partial (\Delta t)^3} \right|_{\Delta t=0} - \left. \frac{\partial^3 \psi_j}{\partial t^3} \right|_{t=0} = -\frac{i}{2\hbar} \left( \left. \frac{\partial^2 h^{(0)}}{\partial t^2} \right|_{t=0} + \frac{i}{\hbar} \left( \left. \frac{\partial h^{(0)}}{\partial t} \right|_{t=0} h^{(0)} - h^{(0)} \left. \frac{\partial h^{(0)}}{\partial t} \right|_{t=0} \right) \right) \psi_j^{(0)} \quad (\text{B.27})$$

From the results of (B.22), (B.25), and (B.27), one sees that the exponential method with the operator defined by (B.15) ensures that the numerical solution obtained at time  $\Delta t$  is equal to the exact solution up to order  $\Delta t^3$ .

A similar analysis made for the CN scheme leads to the same conclusion but with another value for the difference between the exact and numerical third order derivatives. The reason for our choice of the exponential operator was therefore not the better theoretical precision achieved, but the analytical properties of the exponential. Indeed, it is difficult to apply the exact operators  $U_E$  and  $U_{CN}$ .<sup>\*</sup> Instead we use an expansion in powers of  $\Delta t$  for which the exponential always convergent expansion is more appropriate than the expansion of  $1/(1+x)$  associated with the CN method.<sup>†</sup> Two other methods: the alternate direction and the local one-dimensional method have been shown to be equivalent to the CN method up to the order  $\Delta t^3$ .<sup>30</sup> They therefore achieve the same precision as the method used in this paper. However, since the AD and LOD methods do not handle the exact operator  $h^{(\frac{1}{2})}$ , they do not conserve the energy exactly. In addition, the alternate direction method does not use a unitary time propagation operator and does not conserve the norm.

It should be noted that the analysis made in this appendix is restricted to one time step (local error analysis). As far as we know

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<sup>\*</sup>In fact we tested the CN method with the exact inversion performed by means of the conjugate gradient method presented in Appendix C. However, this proved to be more time consuming for a given accuracy than using the expansion of the exponential.

<sup>†</sup>From the above analysis one could be led to believe that an expansion of the exponential up to the order  $\Delta t^3$  is sufficient. However, one has to use more terms in order to conserve both norm and energy (four terms for  $\Delta t = 4 \times 10^{-24}$  s).

there does not exist any rigorous way to estimate the error after a given number of time steps, or better, a given evolution time (global error analysis). In order to estimate the quality of the method used in this paper we have made a calculation of a nuclear collision with two time steps differing by a factor 2 ( $\Delta t = 2$  and  $4 \times 10^{-24}$  s) and checked that the results remained identical up to the fifth figure during and at the end of the collision.

## APPENDIX C: DETERMINATION OF THE COULOMB AND YUKAWA POTENTIALS

The one-body Yukawa and Coulomb potentials are given by Eqs. (8b,c) as convolutions over the nucleon density (recall  $\rho_p = \rho/2$  because of the isospin symmetry we impose). Since these potentials are evaluated many times during each collision (twice per time step), a direct integration of these equations is not possible. We therefore follow the strategy of ref. 12 and calculate the potentials as the solutions of the discrete Poisson and Helmholtz problems

$$\begin{aligned} \nabla^2 W_C &= -2\pi e^2 \rho \quad , \\ \left( \nabla^2 - \frac{1}{a^2} \right) W_Y &= -4\pi V_0 a \rho \quad . \end{aligned} \quad (C.1)$$

Here,  $W_C$ ,  $W_Y$ , and  $\rho$  are column vectors whose components are the values of these functions on the mesh points and  $\nabla^2$  is a sparse matrix approximation to the three-dimensional Laplacian operator.  $W_C$  is a smooth potential due to the long range of the Coulomb force, so that a "three-point" approximation to  $\nabla^2 W_C$  is adequate. However,  $W_Y$  varies relatively rapidly in space and a "five-point" approximation to  $\nabla^2 W_Y$  is necessary (cf. Appendix A).

Given the values of  $W$  on the mesh boundaries (see below), the solution of Eqs.(C.1) amounts to the inversion of a sparse matrix of dimensionality equal to the number of mesh points. It is not possible to invert directly and exactly such a large matrix. We therefore use an iterative method for solving Eqs. (C.1) which construct successive approximations to the solutions and continue the iteration process until sufficient precision is achieved. These methods have the added

advantage that the potentials at the previous time step are excellent starting points for the iteration procedures. Recently an old and rediscovered method, the conjugate gradient method (CGM)<sup>31</sup> has proven to be more rapid than the conventional successive overrelaxation methods and the alternate direction methods.<sup>32</sup> We shall present the CGM for the Poisson equation and discuss briefly the precision achieved. The transposition to the Helmholtz problem is trivial.

Our iterative scheme is a slight modification of that proposed in Ref. 33. At the beginning of the time evolution we start with a first approximation of the potential  $W_C^{(0)}(\vec{r})$  identical to zero.\* At the following time steps we use as a starting point of CGM the last computed value of  $W_C(\vec{r})$ . The calculation of the boundary conditions is discussed at the end of this Appendix. In order to begin the iterative scheme we need two additional vectors,  $Z^{(0)}$  and  $P^{(0)}$ .

$$\begin{aligned} Z^{(0)} &= -\left(2\pi e^2 \rho(\vec{r}) + \Delta W_C^{(0)}(\vec{r})\right) \\ P^{(0)} &= Z^{(0)} \end{aligned} \tag{C.2}$$

The iterative scheme which, in order to save computational time, introduces an additional vector  $T$  and two numbers  $A$  and  $C$ , is then

$$T^{(k+1)} = \Delta P^{(k)} \tag{a}$$

$$A^{(k+1)} = \left(\tilde{Z}^{(k)} \cdot Z^{(k)}\right) / \left(\tilde{Z}^{(k)} \cdot T^{(k+1)}\right) \tag{b} \text{ (C.3)}$$

$$W_C^{(k+1)} = W_C^{(k)} + A^{(k+1)} P^{(k)} \tag{c}$$

---

\*In this Appendix the upper indices  $(k)$  label the number of iterations performed with the CGM method.

C-3

$$Z^{(k+1)} = Z^{(k)} - A^{(k+1)} T^{(k+1)} \quad (d)$$

$$C^{(k+1)} = (\tilde{Z}^{(k+1)} \cdot Z^{(k+1)}) / (\tilde{Z}^{(k)} \cdot Z^{(k)}) \quad (e) \quad (C.3)$$

$$P^{(k+1)} = Z^{(k+1)} + C^{(k+1)} P^{(k)} \quad (f)$$

In formulae (C.3,a-f) the quantity  $(\tilde{Z} \cdot T)$  stands for the scalar product of the two vectors  $Z$  and  $T$ . The method, in addition to its rapidity, provides a natural way to check the convergence. One can show that

$$Z^{(k)} = -\left(2\pi e^2 \rho(\vec{r}) + \Delta W_C^{(k)}(\vec{r})\right) \quad (C.4)$$

so that the norm of the vector  $(k)$  is a measure of the remaining inaccuracy of  $W_C^{(k)}(\vec{r})$ . In our calculation we required this norm to be less than  $10^{-10}$ .

The solution of both Eqs. (C.1) requires a knowledge of the potential boundary conditions. We have assumed that the Yukawa potential is zero at the mesh boundaries. Because of the short Yukawa range ( $a \approx 0.5$  fm), this assumption is valid if there is no appreciable density within about 1 fm of the boundaries. When the system approaches the mesh edges, this boundary condition results in a repulsive image potential and destroys the conservation of the total energy. We have therefore used this phenomenon as a signal for spurious effects from the mesh edges and have stopped the calculation when the total energy was not conserved to within a precision of about 1 MeV.

The long range of the Coulomb potential forces an explicit evaluation of  $W_C$  at the mesh boundaries. Indeed, setting the boundary conditions to zero would result in some 20% error in the Coulomb energy for the box

dimensions used in our calculations. One possibility for evaluating the boundary conditions for  $W_C$  is to evaluate Eq. (8c) at selected points on the box faces by means of Simpson's rule and then compute the remaining boundary conditions by polynomial interpolation. This procedure requires relatively many sweeps of the mesh, but need only be carried out every 3 or 4 time steps. However, a far simpler procedure which is just as accurate is to perform a multipole expansion of the Coulomb potential. If we assume that the system is always separated into two fragments in the way used to define the R coordinate in Section V, then the multipole moments through order three are sufficient to give the required accuracy. This method is advantageous in that it makes use of information which is interesting and would have been computed anyway, the lower multipole moments of the total system and of the fragments.

## REFERENCES

1. P. A. M. Dirac, Proc. Camb. Phil. Soc. 26 (1930) 376.
2. D. J. Thouless and J. G. Valatin, Nucl. Phys. 31 (1962) 11;  
D. J. Thouless, Nucl. Phys. 21 (1961) 225.
3. M. Baranger, in 1962 Cargèse Lectures in Theoretical Physics.
4. M. Baranger, Journal de Physique 33 (1972) C5-61;  
M. Baranger and M. Veneroni, to be published.
5. F. M. H. Villars, in Dynamic Structure of Nuclear States, eds.  
J. J. Rowe et al. (University of Toronto Press, Toronto, 1972), p. 3.
6. D. M. Brink, M. J. Giannoni, and M. Veneroni, Nucl. Phys. A258 (1976) 237.
7. A. K. Kerman, S. E. Koonin, Ann. Phys. N.Y. 100 (1976) 332.
8. Y. M. Engel, et al., Nucl. Phys. A249 (1975) 215.
9. P. Bonche, S. E. Koonin, and J. W. Negele, Phys. Rev. C13 (1976) 1226.
10. R. Y. Cusson and J. Maruhn, Phys. Lett. 62B (1976) 134;  
R. Y. Cusson, R. K. Smith, and J. Maruhn, Phys. Rev. C 36 (1976) 1166.
11. S. E. Koonin, Proceedings of the Workshop IV on Gross Properties of  
Nuclei and Nuclear Excitations, Hirschegg (1976).
12. S. E. Koonin et al., Phys. Rev. C 15 (1977) 1359.
13. V. Maruhn-Rezwani, K. T. R. Davies, and S. E. Koonin, Phys. Lett. 67B  
(1977) 134.
14. P. Bonche, Proceedings of the Workshop IV on Gross Properties of  
Nuclei and Nuclear Excitations, Hirschegg (1976).
15. J. Maruhn and R. Y. Cusson, Nucl. Phys. A270 (1976) 437.
16. R. Y. Cusson, J. A. Maruhn, and H. W. Meldner, to be published.
17. A. K. Kerman, in Proceedings of the Enrico Fermi Summer School,  
Varenna (1976).
18. P. Bonche, Proceedings of the Caen Conference on Heavy Ions, Caen (1976).



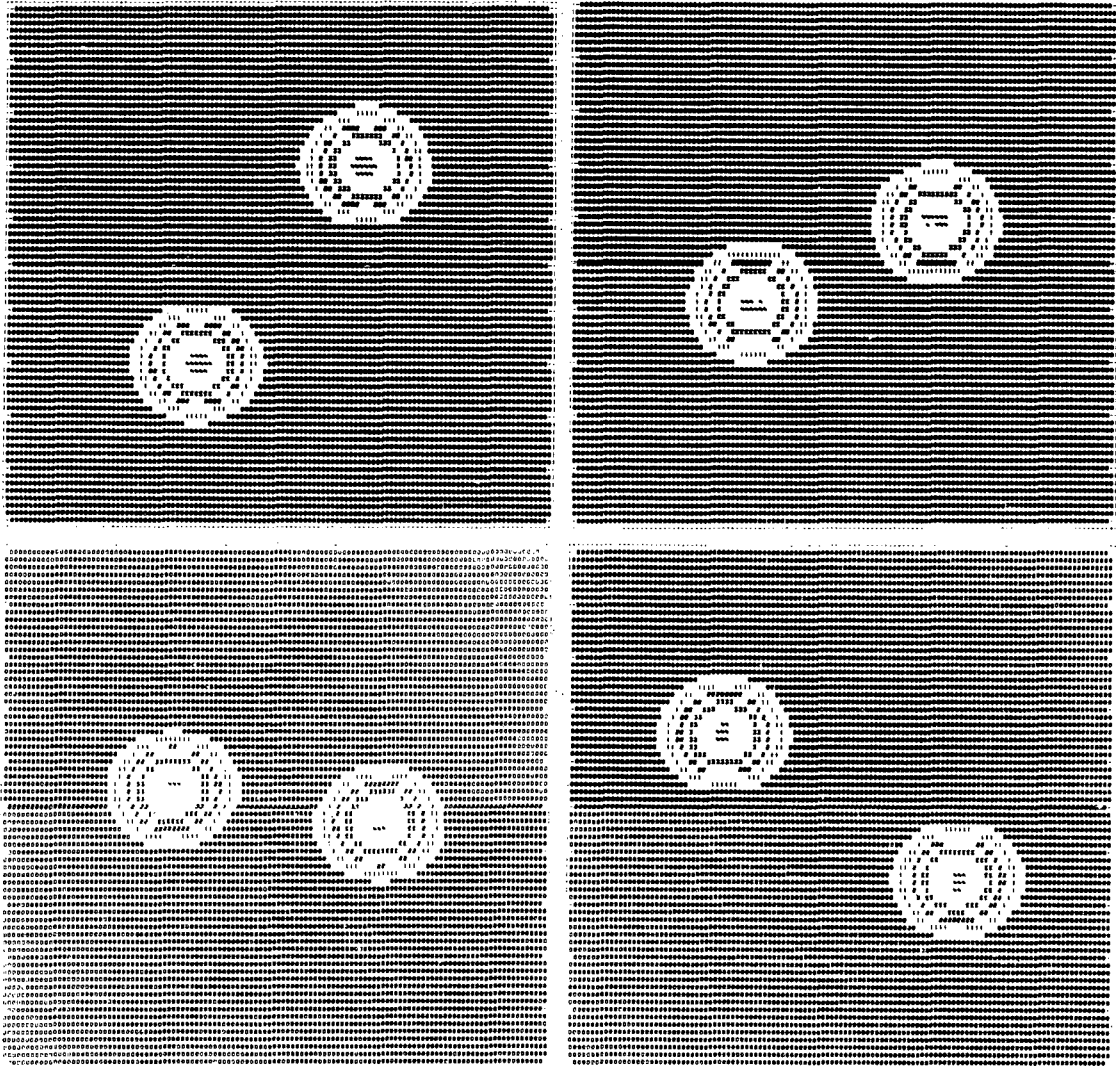
19. P. Bonche, B. Grammaticos, and S. E. Koonin, to be published.
20. V. M. Strutinsky, Nucl. Phys. A95 (1967) 420;  
V. M. Strutinsky, Nucl. Phys. A122 (1968) 1;  
M. Brack, Int. School of Nucl. Phys., Predeal, Romania (1974);  
V. M. Strutinsky, Nucl. Phys. A218 (1974) 169.
21. W. J. Swiatecki, LBL Report No. 4296, unpublished, presented at the international school seminar on reactions of heavy-ions with nuclei and synthesis of new elements, Dubna, USSR (1975).
22. C. Y. Wong, J. A. Maruhn, and T. A. Welton, Nucl. Phys. A256 (1975) 469; Phys. Lett. 66B (1977) 19.
23. M. J. Giannoni, D. Vautherin, M. Veneroni, and D. M. Brink, Phys. Lett. 63B (1976) 8.
24. D. Vautherin, Comptes rendus de la troisieme session d'etudes biennale de la Toussuire, ed. El. Baz (1975).
25. Goldberger and Watson, Collision Theory (John Wiley & Sons, 1964).
26. See, for example, M. A. Preston, R. K. Bhaduri, Structure of the Nucleus (Addison Wesley, 1975), 357 pp.  
A. Bohr and B. R. Mottelson, Nuclear Structure II, ed. W. A. Benjamin (1975), 667 pp.
27. H. Flocard, Phys. Lett. 49B (1974) 129.
28. P. Sperr et al., Phys. Rev. Lett. 36 (1976) 405;  
P. Sperr et al., Phys. Rev. Lett. 37 (1976) 321;  
B. Fernandez et al., to be published.
29. M. Abramowitz and I. Stegun, Handbook of Mathematical Functions (National Bureau of Standards, 1965), 884 pp.
30. A. R. Mitchell, Computational Method in Partial Differential Equations (John Wiley & Sons, New York, 1965).

31. J. Reid, *SIAM J. Num. Anal.* 9 (1972) 325.
32. R. Varga, Matrix Interactive Analysis (Prentice Hall, Englewood Cliffs, 1962) 273 pp.
33. P. Concus, G. H. Golub, and D. P. O'Leary, Sparse Matrix Computations, eds. J. R. Bunch, D. J. Rose (Academic Press, 1976);  
P. Concus, G. H. Golub, and C. W. Nielson, *SIAM J. Num. Anal.* 7  
(1970) 627.

FIGURE CAPTIONS

- Fig. 1. Contour lines of the density integrated over the coordinate normal to the scattering plane for an  $^{16}\text{O} + ^{16}\text{O}$  collision at  $E_{\text{lab}} = 105$  MeV and incident angular momentum  $L = 40\hbar$ . The time interval between two pictures is  $2 \times 10^{-22}$  s.
- Fig. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an  $^{16}\text{O} + ^{16}\text{O}$  collision at  $E_{\text{lab}} = 105$  MeV and incident angular momentum  $L = 13\hbar$ . The times  $t$  are given in units of  $10^{-22}$  s.
- Fig. 3. Contour lines of the density integrated over the coordinate normal to the scattering plane for an  $^{16}\text{O} + ^{16}\text{O}$  collision at  $E_{\text{lab}} = 105$  MeV and incident angular momentum  $L = 5\hbar$ . The times  $t$  are given in units of  $10^{-22}$  s.
- Fig. 4. Trajectories of the vector separation,  $\vec{R}$ , between the centers-of-mass of the two fragments for incident angular momentum values ranging from 0 to  $40\hbar$ .
- Fig. 5. Examples of different trajectories leading to fusion.
- Fig. 6. Trajectory for a nearly head-on ( $L = 0.5\hbar$ ) collision at low energy ( $E_{\text{lab}} = 32$  MeV) which leads to fusion.
- Fig. 7. Contour lines of the density integrated over the coordinate normal to the scattering plane for an  $^{16}\text{O} + ^{16}\text{O}$  collision at  $E_{\text{lab}} = 192$  MeV and incident angular momentum  $L = 42\hbar$ . The time interval between two pictures is  $10^{-22}$  s.
- Fig. 8. Deflection angle and kinetic energy loss as a function of incident angular momentum at  $E_{\text{lab}} = 105$  MeV. The shaded area corresponds to the fusion window.

- Fig. 9. Schematization of the nuclear part of a heavy-ion potential.  $E_\infty$  is the kinetic energy for infinitely separated fragments. The dashed line is a trajectory in the absence of dissipation. It is shifted from  $E_\infty$  by the point Coulomb energy  $E_C$ . The solid line is a trajectory with dissipation and  $W$  stands for the energy loss.
- Fig. 10. Time-dependent single-particle energy spectrum (see text) for a nearly head-on collision ( $L = 0.5\hbar$ ,  $E_{lab} = 105$  MeV).
- Fig. 11. Upper part: the point Coulomb energy  $E_C$  and the mechanical energy  $E_M$  (see text) as a function of time for a nearly head-on collision ( $L = 0.5\hbar$ ,  $E_{lab} = 105$  MeV). Lower part: the corresponding time evolution of the fragment separation coordinate.
- Fig. 12. The thick lines indicate the box in which the calculations are actually performed and the thin lines the complete box deduced by means of the two imposed symmetries. The gray surface indicates a possible equidensity contour surface with the same convention.
- Fig. 13. Relative error in the kinetic energy of the lowest state of an oscillator. The results are shown for the five-point and three-point formulae of the kinetic energy and different mesh sizes. The oscillator parameter is  $m\omega/\hbar = 0.275$  fm<sup>-2</sup>.



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Figure 1

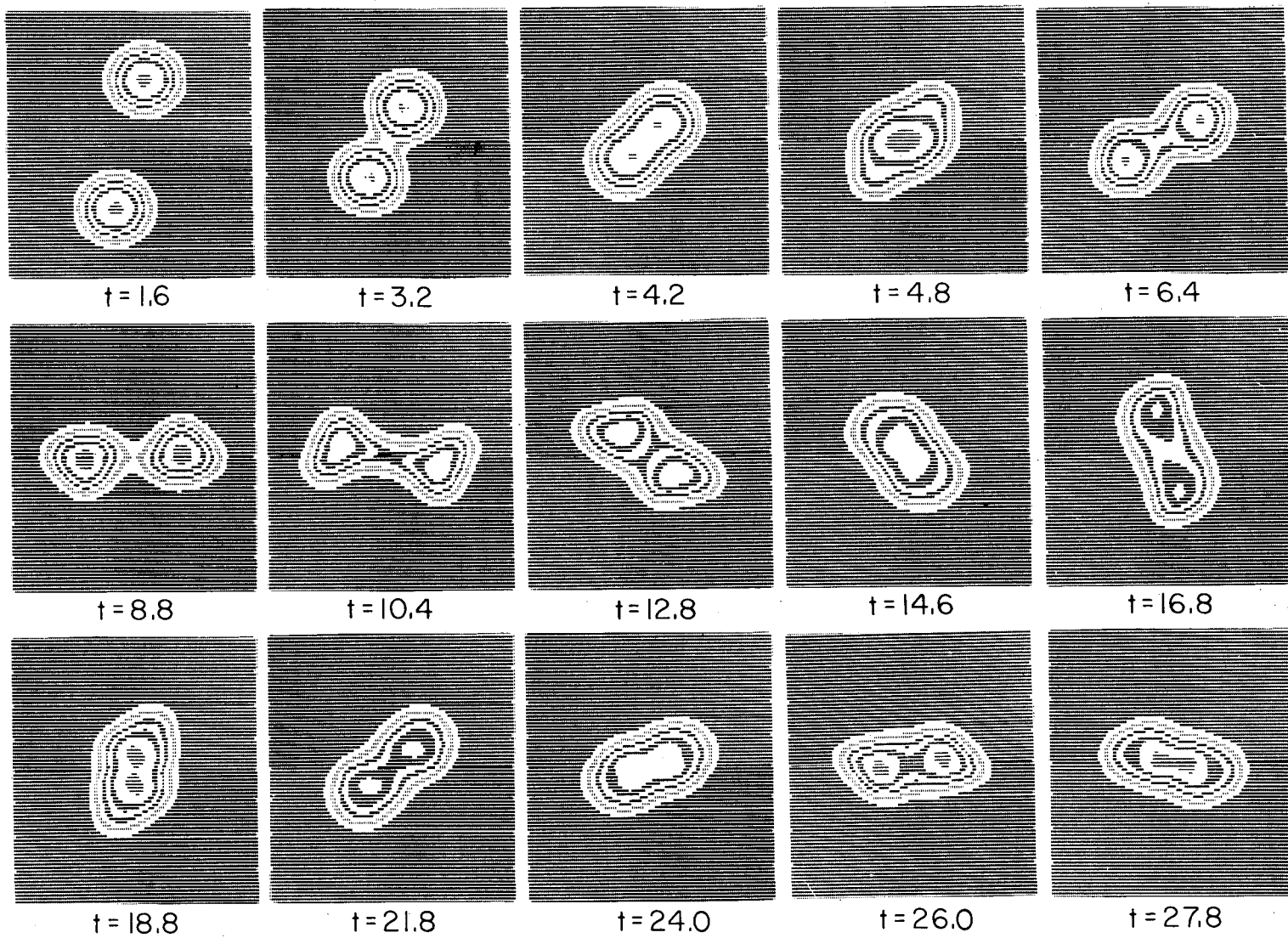
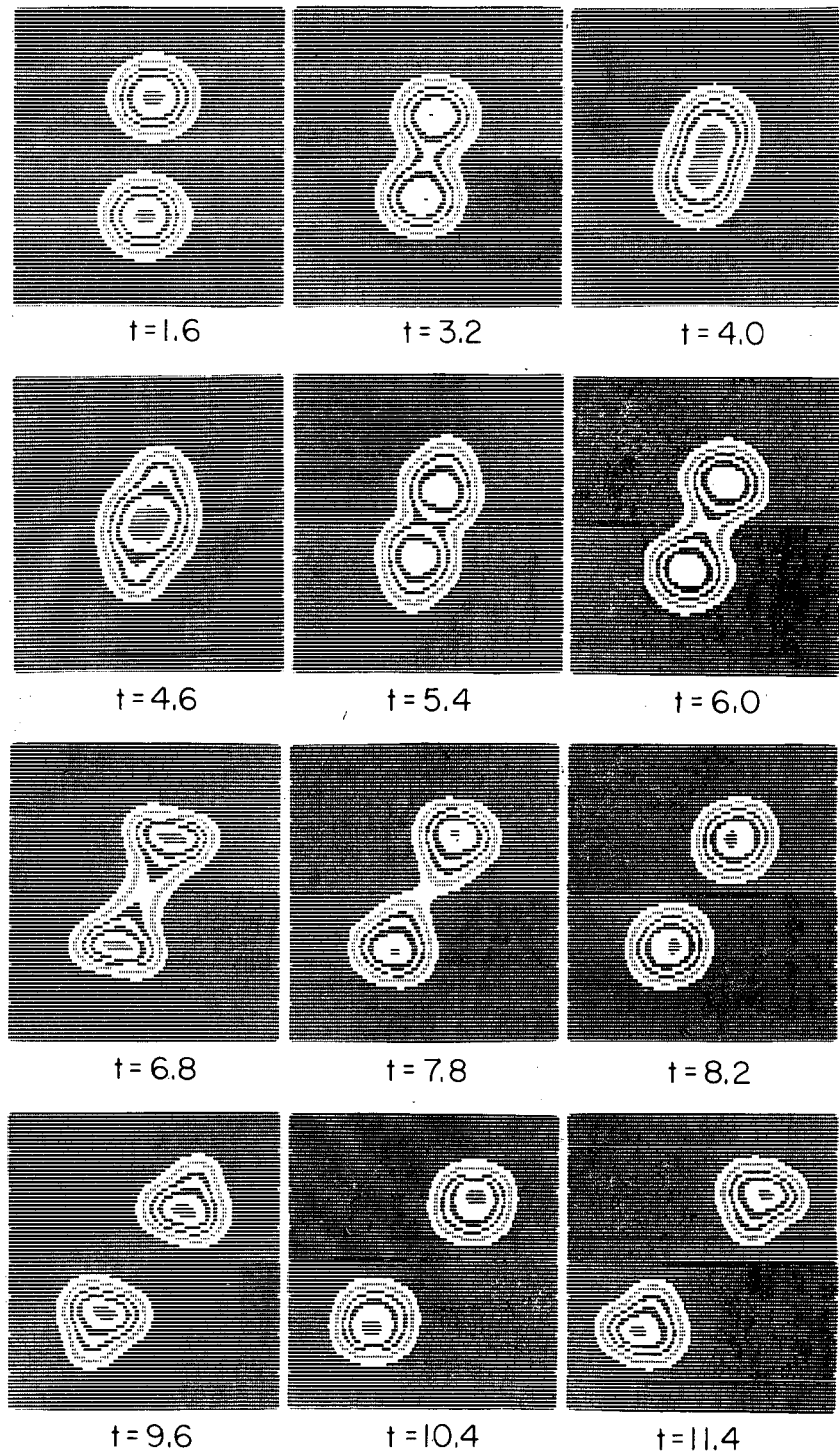


Figure 2

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Figure 3

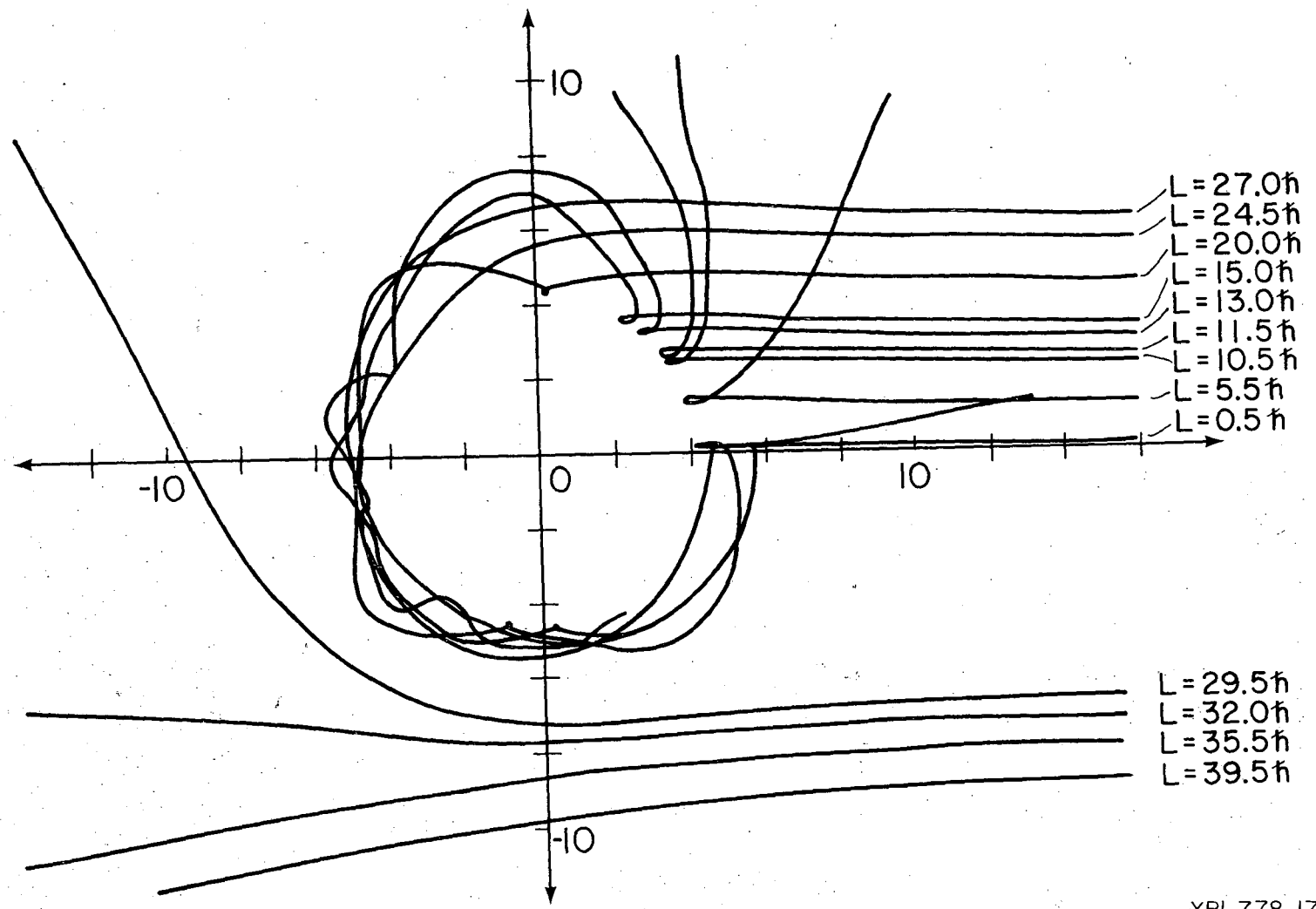


Figure 4

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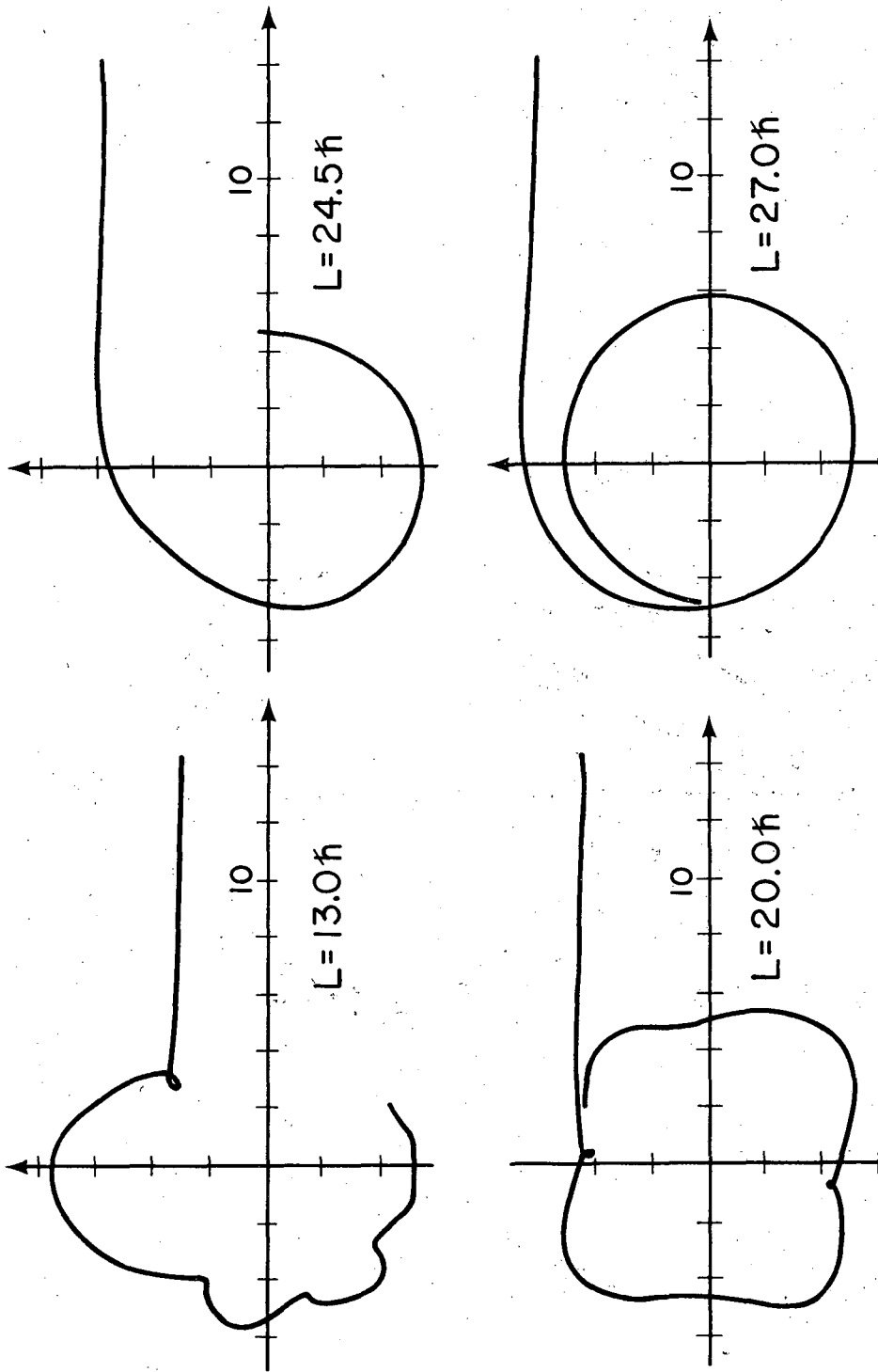
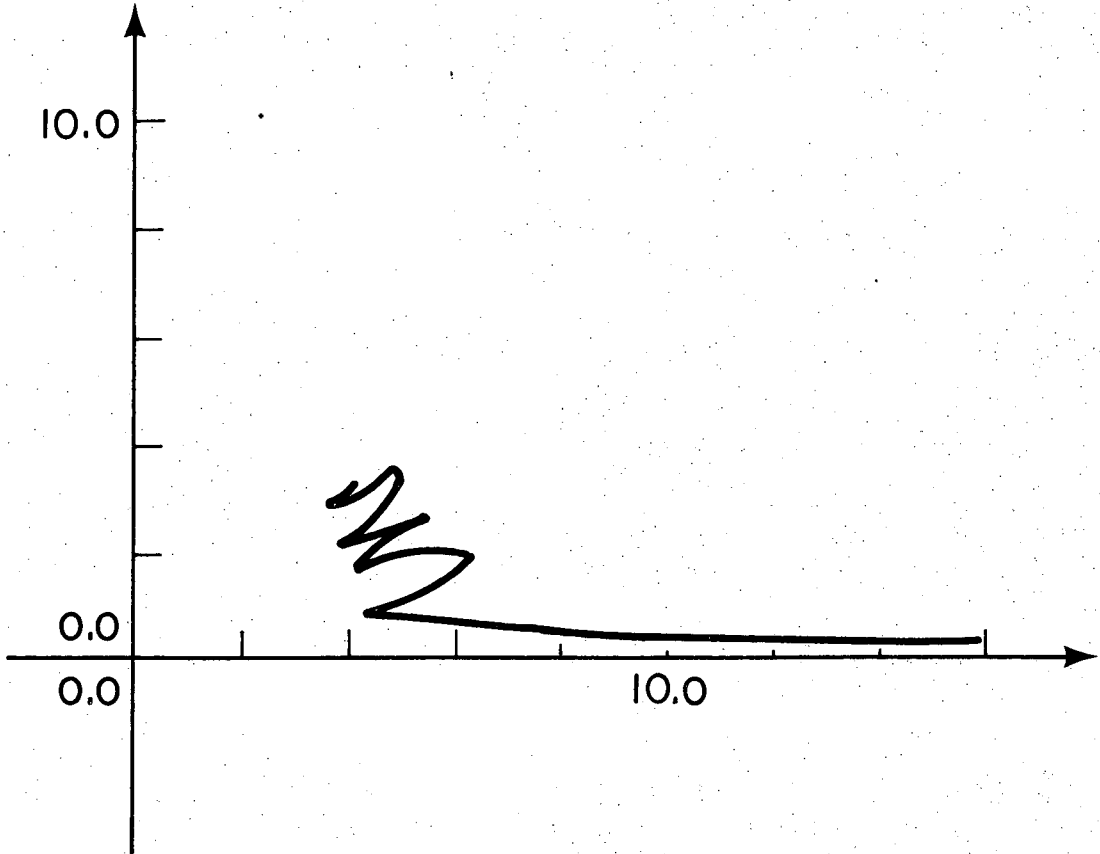


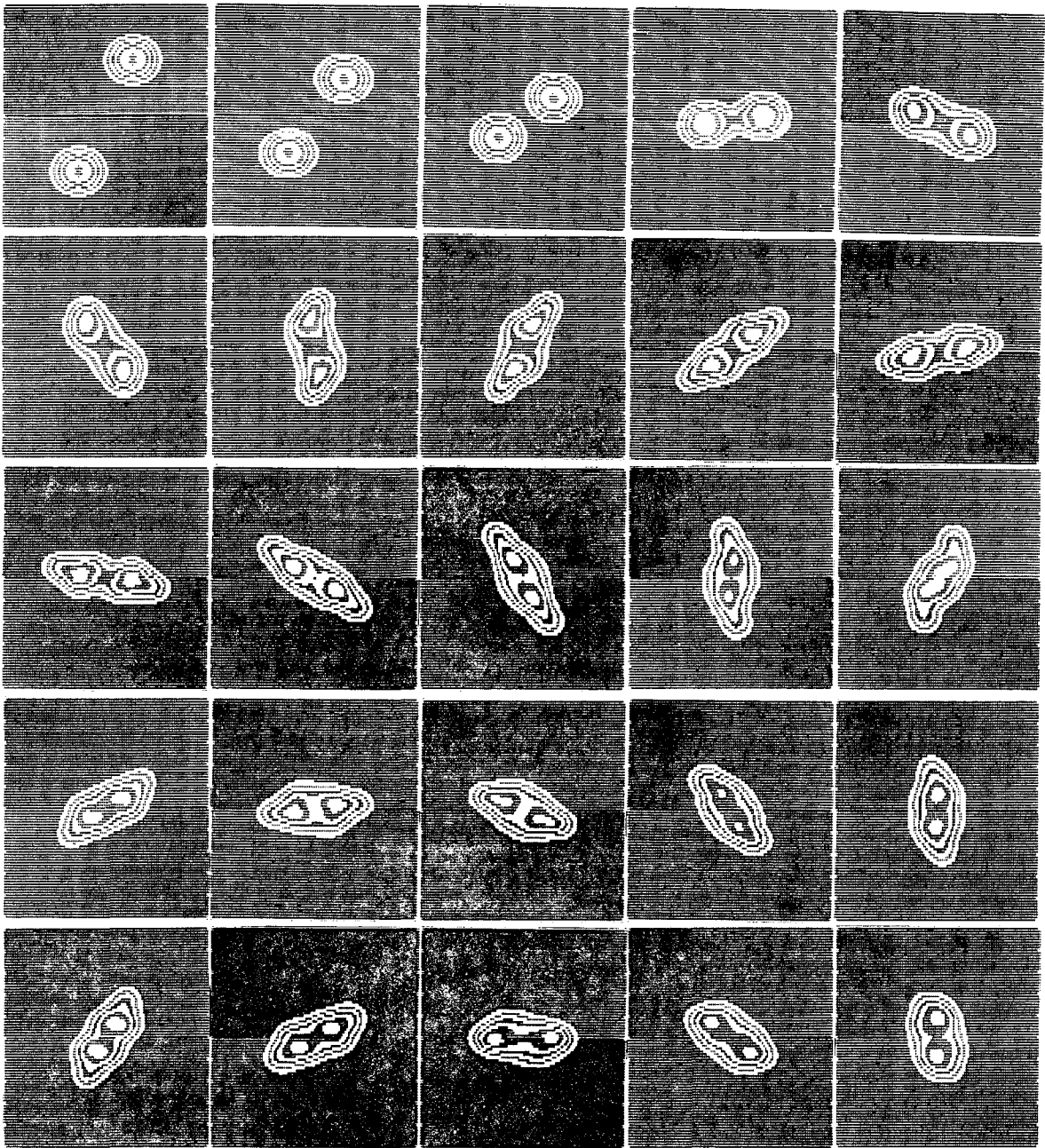
Figure 5

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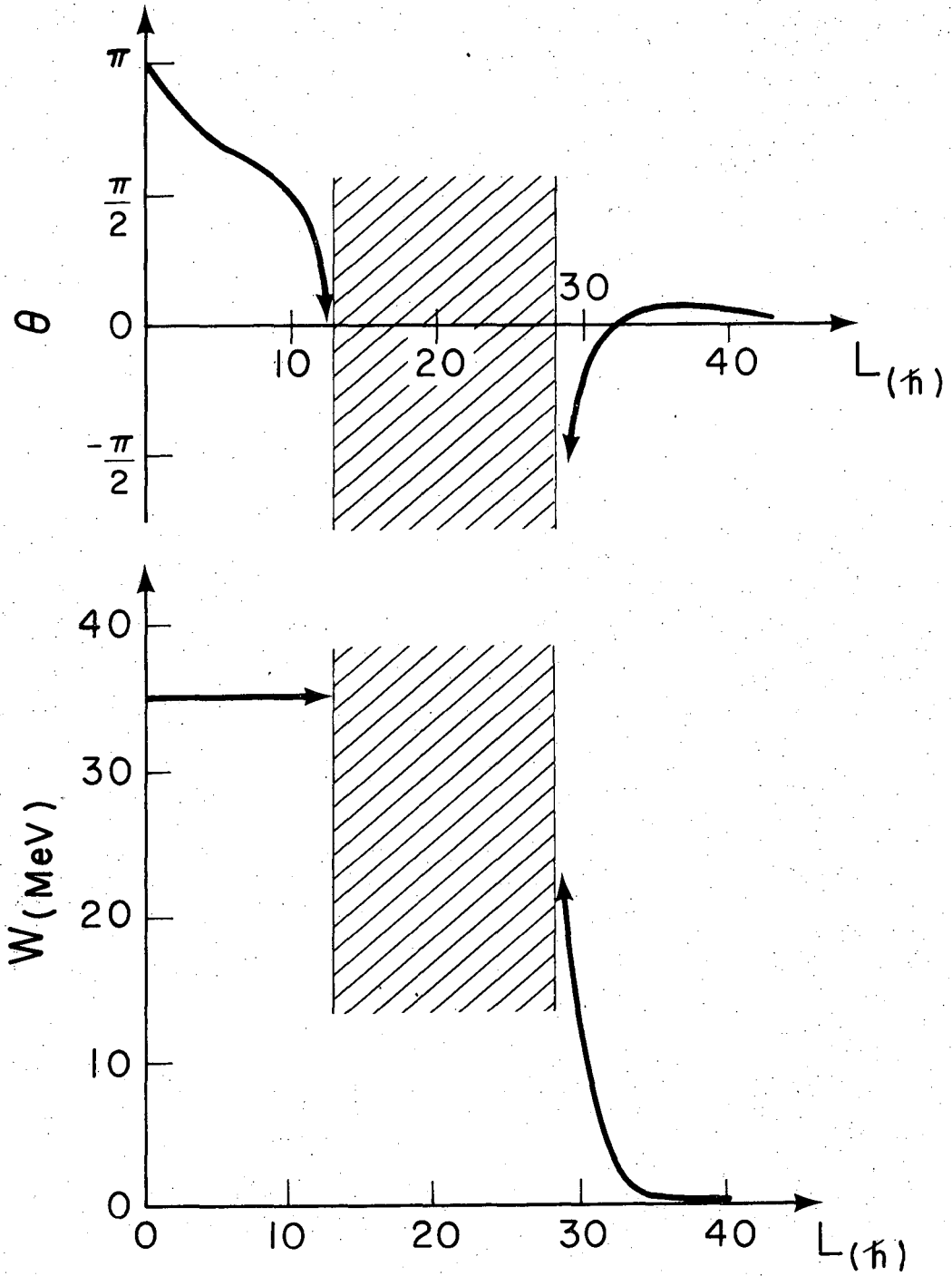
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Figure 6



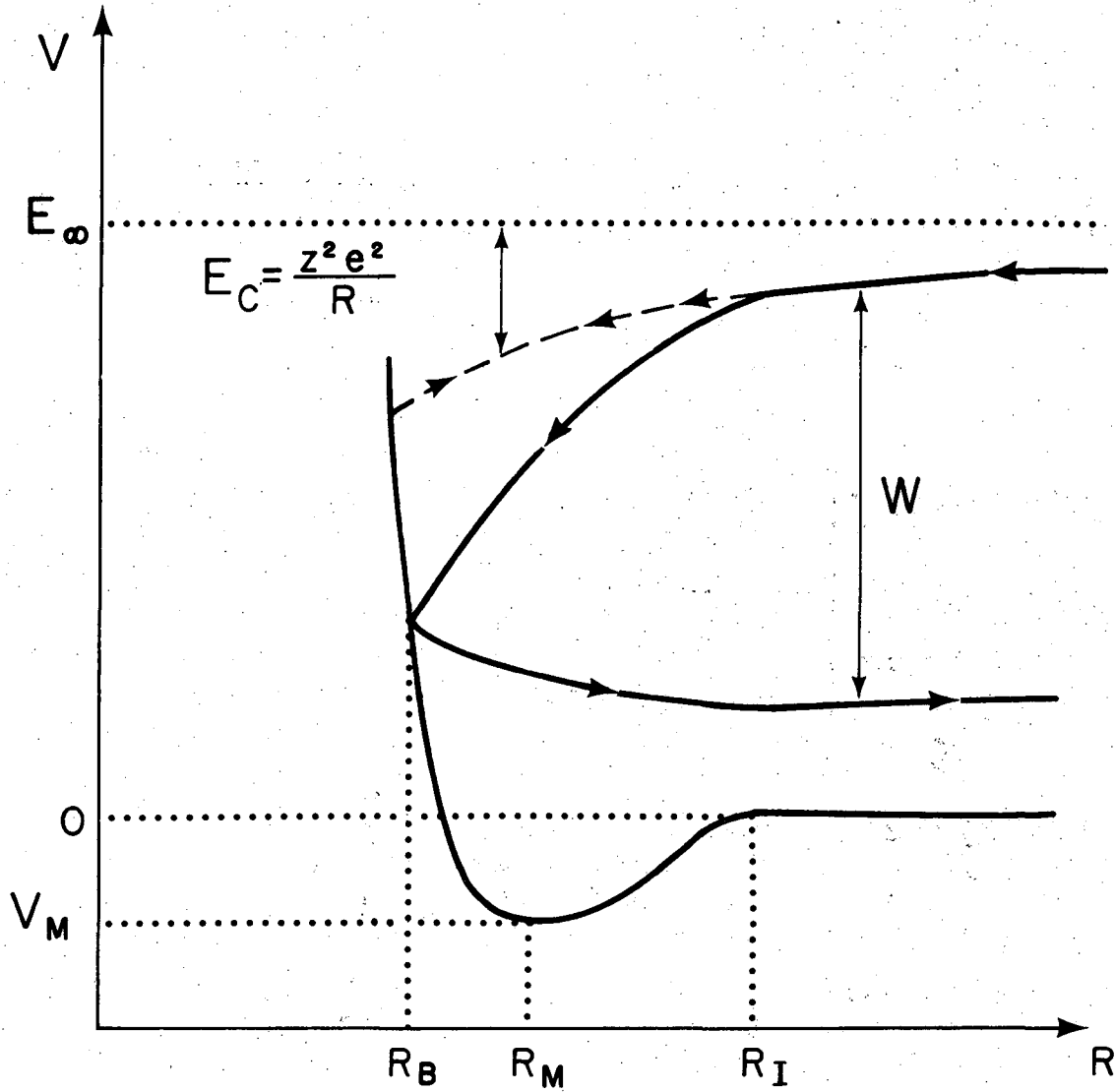
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Figure 7



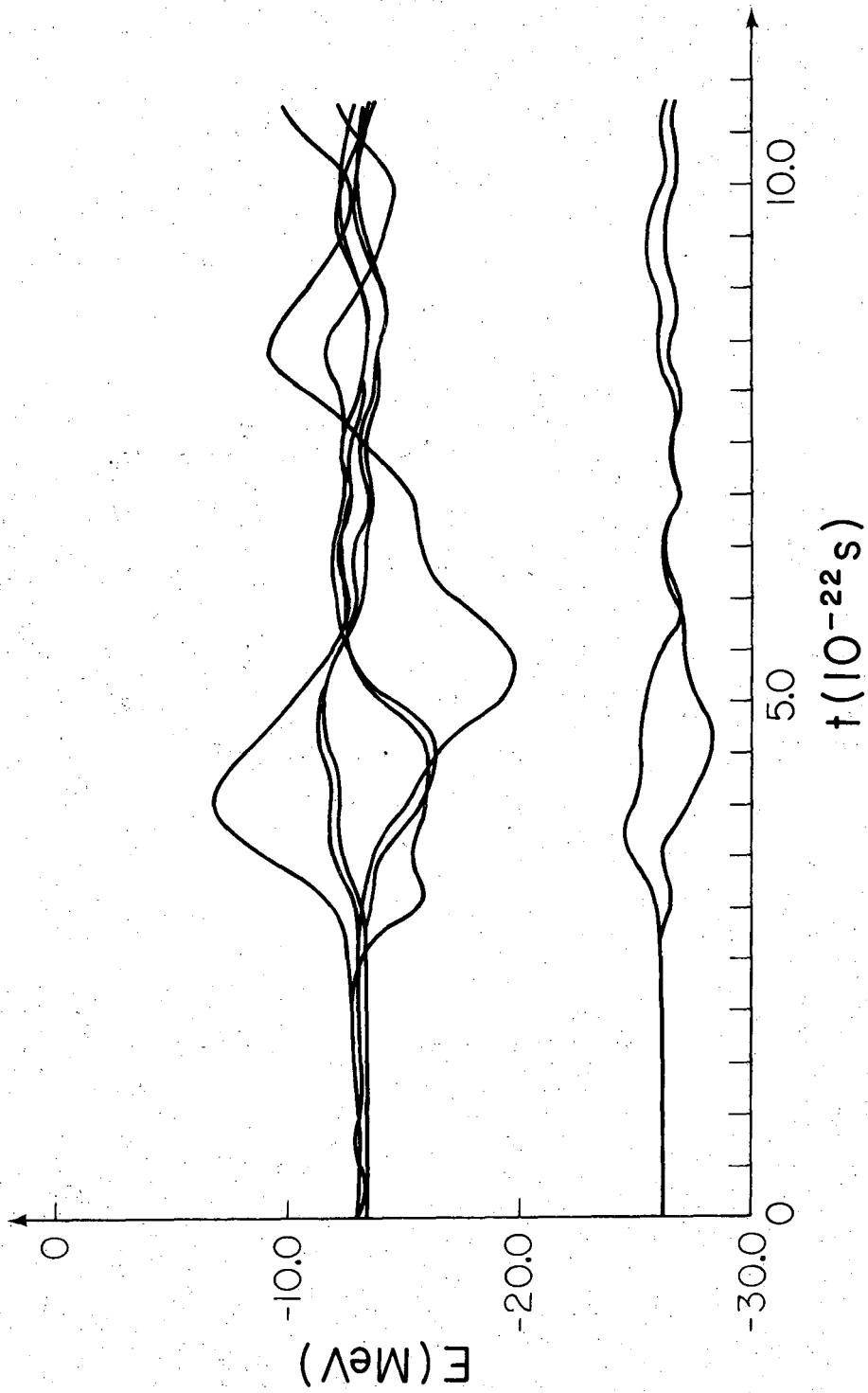
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Figure 8



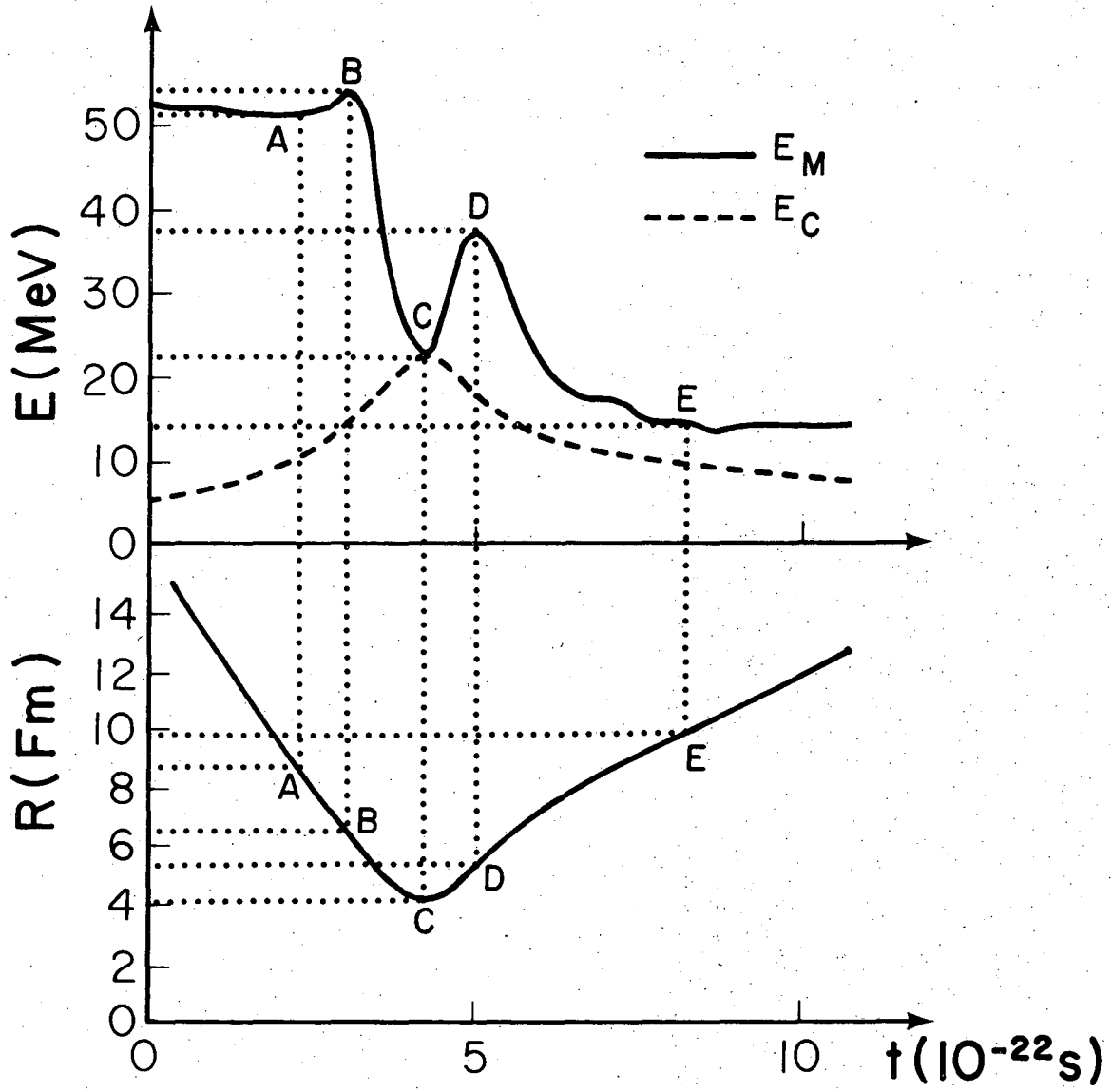
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Figure 9



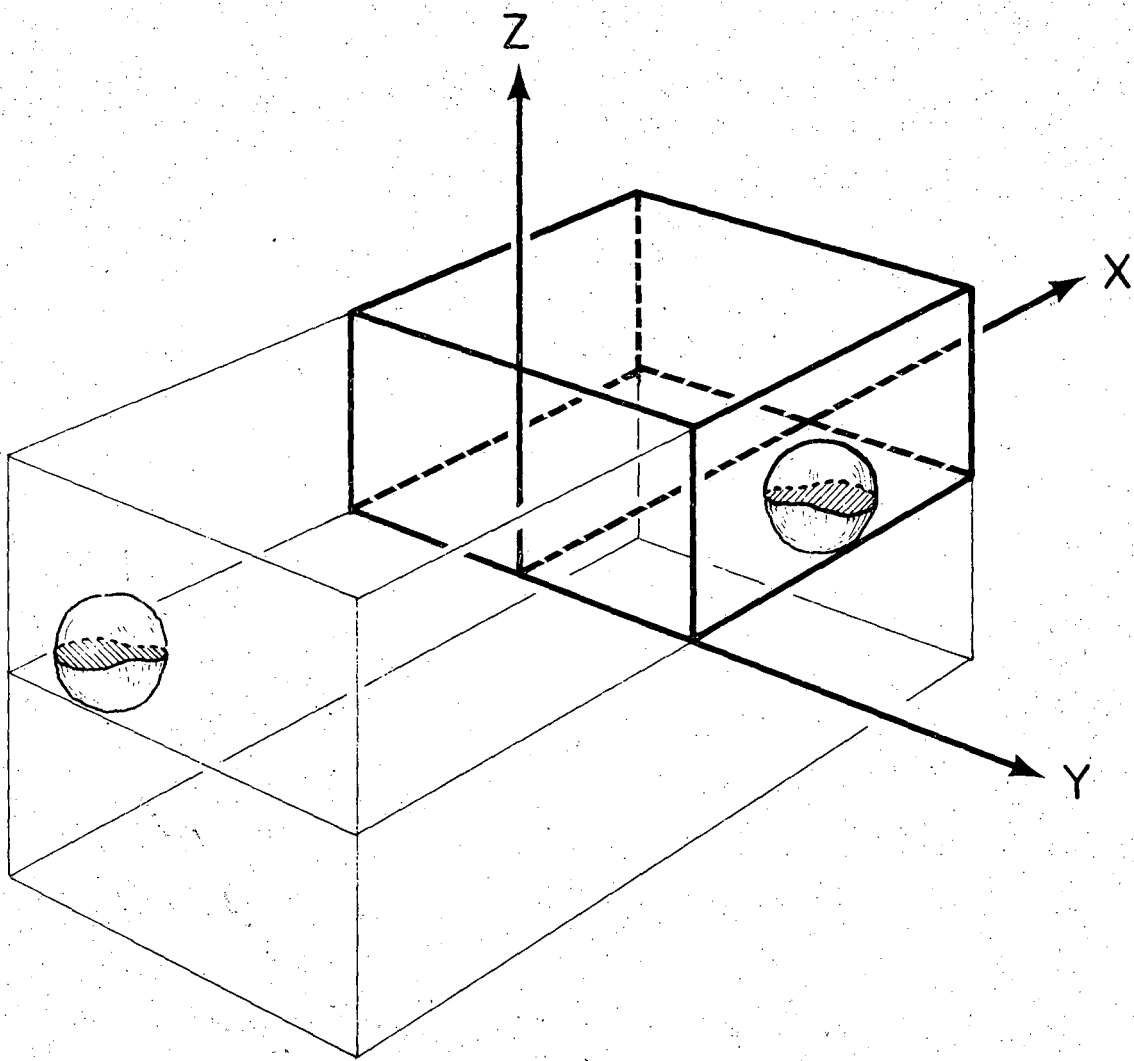
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Figure 10



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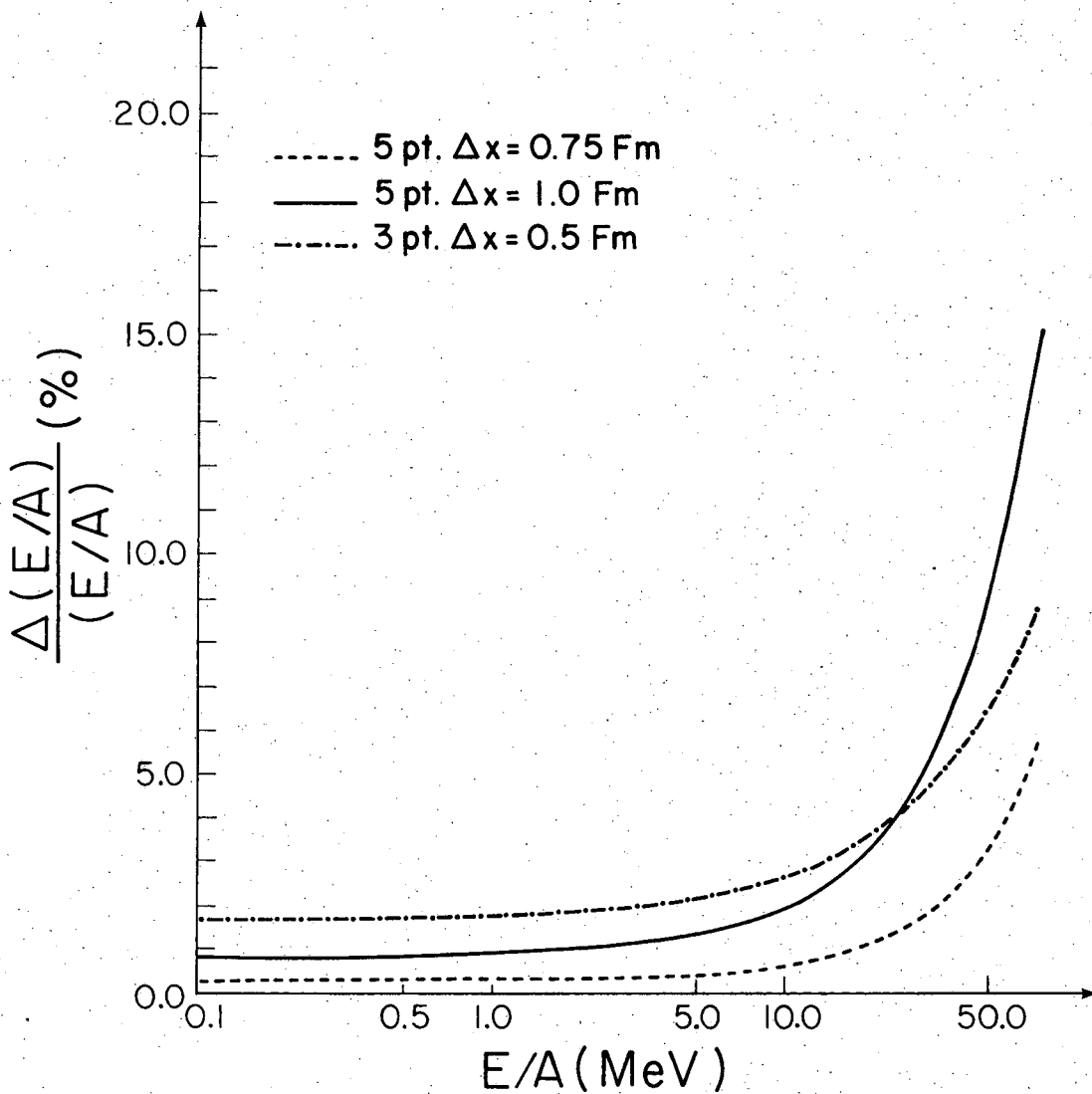
Figure 11



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Figure 12





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Figure 13

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