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Time-Dependent Hartree-Fock Calculation of the Reaction $^{16}O + ^{16}O$ in Three Dimensions

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We have solved the time-dependent Hartree-Fock equations in three dimensions for the heavy-ion reaction $^{16}O+^{16}O$ at energies $E_{lab}/A_{proj}=8$, 16, and 24 MeV and impact parameters $b=0$, 2, 4, 6, and 8 fm. The potential used is a simplified form of the Skyrme interaction. An angular-momentum window for complete fusion is predicted. A multifluid flow pattern similar to that of atomic physics is observed and seems to cast doubts on the validity of the simplified axiality and rigid clutching assumptions currently made.

The time-dependent Hartree-Fock (TDHF) formalism[1] has been found to yield encouraging results in the calculation of head-on (two-dimensional) collisions of nuclear heavy ions such as $^{12}C+^{12}C$[2] and $^{16}O+^{16}O$.[3] Much more interesting results on reaction cross sections require, however, that the ions collide with a finite impact parameter in the semiclassical context implied by the single-Slater-determinant nature of the TDHF prescription. One must therefore do a complete three-dimensional calculation or make simplifying assumptions[4] concerning the behavior of the collision in a rotating frame. It is important to check these assumptions by doing the more complete calculation. We have therefore solved the TDHF equations discussed below, on a three-dimensional grid consisting of $16\times24\times24$ points with a spacing of 1 fm, for the reaction $^{16}O+^{16}O$, at various energies and impact parameters given in Table I. We first describe briefly the combined techniques of fast Fourier transform and predictor-corrector method used to solve the Schrödinger equation. We then discuss our results and finally we point out their implication for heavy-ion calculations and for the search of a rotating-frame simplified model.

The TDHF model assumes that the time-dependent wave function of the colliding ions is given by a single Slater determinant whose occupied single-particle orbits $\psi_\lambda(\vec{r},t)$ obey the TDHF single-particle Schrödinger equation

$$i\hbar\frac{\partial\psi_\lambda(\vec{r},t)}{\partial t}=h\psi_\lambda(\vec{r},t),\quad \lambda=1,\ldots,A_1+A_2, \tag{1}$$

where A_1 and A_2 are the number of particles in each ion and h is the single-particle Hamiltonian which we have taken for simplicity as

$$h=\hbar^2k^2/2m-a\rho(r)+b\rho^2(r), \tag{2}$$

with $a=+817.5$ MeV fm^3 and $b=3241.5$ MeV fm^6. These two parameters correspond to a simplified version of the Skyrme interaction,[1,3] while the first term is the free kinetic energy operator. We assume $Z=N$ and spin saturation so that each space wave function applies to four nucleons; thus

$$\rho(r,t)=4\sum_{\lambda=1}^{N_1+N_2}|\psi_\lambda(r,t)|^2. \tag{3}$$

Whereas the potential energy part of h in Eq. (2) is bounded, the kinetic energy is not. The kinetic energy can be removed from the Schrödinger

TABLE I. Summary of results for the heavy-ion reaction $^{16}O+^{16}O$ at various incident energies and impact parameters.

Incoming E_{lab}/A_{proj} (MeV)	Impact parameter b (fm)	Max. nonaxiality γ [a] (deg)	k_{rel} (fm^{-1})	E_{col}(in, c.m.) (MeV)	E_{col}(out, c.m.) (MeV)	$R_{rms}^{(min)}$ [b]	$t(R^{min})$ (fm/c)	θ_{scat} (deg)	$\hbar^{-1}L$(c.m.)
16	0	0	0.879	128	42	3.17	40	0 (180)	0
16	2	−16.1	0.879	128	38	3.22	40	65 (115)	14.1
16	4	−57	0.879	128	30	3.41	45	... [c]	28.1
16	6	− 9.2	0.879	128	37	3.94	45	60	42.2
16	8	0	0.879	128	117	4.76	32	1	56.3
8	6	− 9.1	0.621	64	30	3.75	142	25	29.8
24	6	− 8.2	1.076	192	90	3.95	37	19	51.6
24	4	−48.6	1.076	192	28	3.39	38	115	34.4

[a] We use $\langle R_\nu^2\rangle = \langle R_0^2\rangle_{av} \exp[(5\pi^{-1})^{1/2}\beta\cos(\gamma - \frac{2}{3}\nu\pi)]$, $\nu = 1,2,3$; $\langle R_0^2\rangle_{av} = (\langle R_x^2\rangle\langle R_y^2\rangle\langle R_z^2\rangle)^{1/3}$.

[b] The rms radius of the $A=32$ system in its ground state would be ~ 3.15 fm.

[c] After $t = (300\text{ fm})/c$, the system is still bound and has effectively captured. The scattering angle is indeterminate and this value of b is omitted from the cross-section calculation mentioned in the text.

equation (1), however, by working in momentum space and inserting a phase factor $\exp(-i\hbar k^2 t/2m)$ into the momentum-space wave function. The transformation from coordinate to momentum space is obtained as

$$\psi_\lambda(k_\nu, t) = \frac{1}{N}\sum_{J=0}^{N-1}\psi_\lambda(x_\epsilon, t)e^{-2\pi i\epsilon\nu/N}, \qquad \nu = -\tfrac{1}{2}N, \ldots, +\tfrac{1}{2}N - 1, \tag{4}$$

in the x direction. A triple sum is used in three dimensions. The grid points x_ϵ and k_ν are obtained as

$$x_\epsilon = \epsilon\Delta x, \quad k_\nu = 2\pi\nu/L, \qquad \Delta x = 1\text{ fm}, \quad L = N\Delta x. \tag{5}$$

The sums in Eq. (4) are performed efficiently by using a fast-Fourier-transform algorithm.[5] The Schrödinger equation is actually solved in momentum space and one comes back to coordinate space only in order to perform $v(\rho(r))\psi_\lambda$. We have used 16 points in the x direction and 24 points in the y and z directions. The y-z plane is taken to be the scattering plane. We enforce a symmetry about the plane $x=0$, so that all wave functions are either even or odd under $x \to -x$. We also truncate the momentum space to states which have a total kinetic energy of less than 125 MeV. This results in a momentum space having 1287 components. Equation (1) is integrated in time by taking fixed time steps of $\Delta t = (1.25\text{ fm})/c$ [$(1\text{ fm})/c = 3.33\times10^{-24}$ sec] and using a seventh-order predictor-corrector formula.[6] The expectation value of the total energy and the unity of the normalization are preserved to 1 part in 10^5 at each time step.

The initial wave function for each ^{16}O ion is constructed by using real harmonic-oscillator wave functions with an oscillator parameter[3] of 1.668 fm. These real wave functions are then multiplied by the phase factor $\exp(\pm i\vec{k}\cdot\vec{r})$, where $\vec{k}$ is the collective momentum in the c.m. system of the particles in each cluster. We have $\vec{k} = \frac{1}{2}\vec{k}_{rel}$, with $\vec{k}_{rel}$ the relative momentum given in Table I. The energy per nucleon is the laboratory energy of the projectile divided by the atomic number of the projectile and is related to $\vec{k}_{rel}$ by $E_l/A_p = \hbar^2|k_{rel}|^2/2M_p$, for a target at rest. E_l/A_p is also given in Table I. The ions are started at 10 fm from each other and the impact parameter b is the distance of closest approach of the two c.m.'s of the ions in the absence of interactions. The collective energy is defined as earlier[2] by $E_{col} = \int d^3r\, \frac{1}{2}m|\vec{J}(\vec{r})|^2/\rho(\vec{r})$, with $\vec{J}$ and $\rho(r)$ the total probability current and density. The total angular momentum in the c.m. system is obtained from the usual expression $L_{c.m.} = \hbar\mu k_{rel} b$, with $\mu = A_1A_2/(A_1+A_2)$.

Table I summarizes our results for the $^{16}O+^{16}O$ case. The nonaxiality angle is computed in the principal-axis frame, e.g., the rotated frame in the y-z plane where the mass quadrupole moment is diagonal. The value $\gamma = 0°$ corresponds to an axial configuration in that frame, while an angle of 60° corresponds to a configuration whose mass-quadrupole ellipsoid is axially symmetric around the x direction, e.g., *perpendicular* to the scattering plane. The time at which the rms

mass radius of the whole system attains its minimum value is given in Table I, together with the value $R_{\rm rms}$ at the minimum. Since these values are all greater than the one, 3.15 fm, that the compound system would have in its ground state, we see that none of the cases presented here show any degree of compression beyond the usual equilibrium nuclear-matter values. The scattering angle is obtained by observing the direction of motion of the clusters after they separate. During the scattering it is usually not possible to identify two separate clusters.

At $E_l/A_p = 16$ MeV the quoted values of $\theta_{\rm scat}$ versus b lead to an approximate differential cross section of the form $d\sigma/d\Omega = 0.5\,\partial b^2/\partial\cos\theta \approx 16$ fm^2, when the identical nature of the two particles is taken into account. This corresponds to a total inelastic cross section of 2 b. One should exercise caution in comparing this result with experiment, however, because we have not corrected for Coulomb effects and nucleon evaporation during the scattering; we also have few points to work with. The table also shows the collective energy loss versus impact parameter at $E_l/A_p = 16$ MeV. The smallest outgoing energy is observed at $b = 4$ fm mainly because the long contact interval allows more time to transform the collective energy into internal (incoherent) kinetic energy (heat!). For smaller values of E_l/A_p, this would lead to an impact-parameter or angular-momentum window for complete fusion. The time delay suffered by the collision can be observed by comparing the various energies at $b = 6$ fm. For $E_l/A_p = 8$, 16, and 24 MeV, we find $t(R^{\rm min}) = (142, 37,$ and 32 fm$)/c$, respectively. The scattering at $E_l/A_p = 8$ MeV should have a $t(R^{\rm min}) = (55$ fm$)/c$ if it scaled as $1/k_{\rm rel}$, whereas an additional delay of (87 fm)$/c$ is observed before the minimum radius is achieved. This additional delay should greatly enhance evaporation effects and hence increase the subsequent complete fusion due to energy losses by evaporation. We also note that the radius never becomes smaller than 3.15 fm, the rms radius of the ground state of the $A = 32$ compound system. This indicates that compression effects play no role at these energies ($K_{\rm nuclear\ matter} = 364$ MeV, here).

A more detailed account of the event at $E_l/A_p = 24$ MeV, $b = 4$ fm, is given in Fig. 1, where several quantities are plotted as a function of time. The integrated central density $\rho_{\rm cent}{}^I = \int dx \times \rho(x, y = 0, z = 0)$ is shown and is seen to go to zero only after about (200 fm)$/c$, which is very

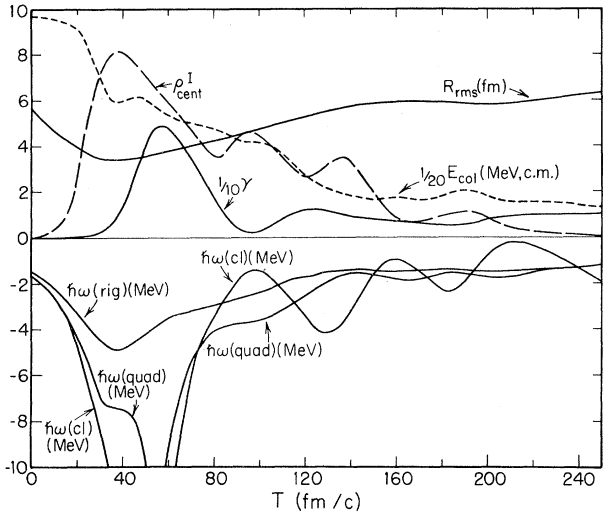

FIG. 1. Time development of several parameters of the reaction $^{16}O + {}^{16}O$ at $E_l/A_p = 24$ MeV, $b = 4$ fm [$\hbar^{-1} \times L$(c.m.) = 34.4]. cl denotes cluster. γ is in degrees.

much longer than the (38 fm)$/c$ it takes to achieve minimum radius. The behavior of the system during this second half of the collision is complex. We illustrate some of the events in Fig. 2 which shows equidensity contours of $\rho^I(y, z)$ at various times. It appears that after the main collision, various fractions of the nuclear liquid rotate in the scattering plane with different angular velocities. This is a well-known effect in atomic scattering where the nuclei and the atomic clouds may have very different angular velocities. Thus during the region of maximum asymmetry near $t = (60$ fm$)/c$ we have a flattened system ($\gamma \approx 60°$) with a high-density inner portion rotating much faster than the lower-density outer bumps. In such a multifluid flow pattern the angular velocity of rotation of the total mass-quadrupole-moment ellipsoid is erratic and may even change sign. For the case shown in Fig. 2, $\hbar\omega$(quad) shows wide fluctuations compared to the rigid angular velocity defined as $\hbar\omega(\text{rigid}) = \hbar L/I_{\rm rigid}$, with $I_{\rm rigid}$ the usual rigid-body moment of inertia about the x axis. Figure 2 also shows a cluster angular velocity defined as the angular velocity of the center of mass of the orbits which originally constituted the first fragment. This velocity is meaningful only as long as these orbits remain clustered around one or the other fragment, something which fails at some values of E_l/A_p and b, but which is nearly true in Fig. 2.

The present calculation would indicate that the two fragments have clutched and rotated as a common rigid entity whenever $\hbar\omega$(rigid) and

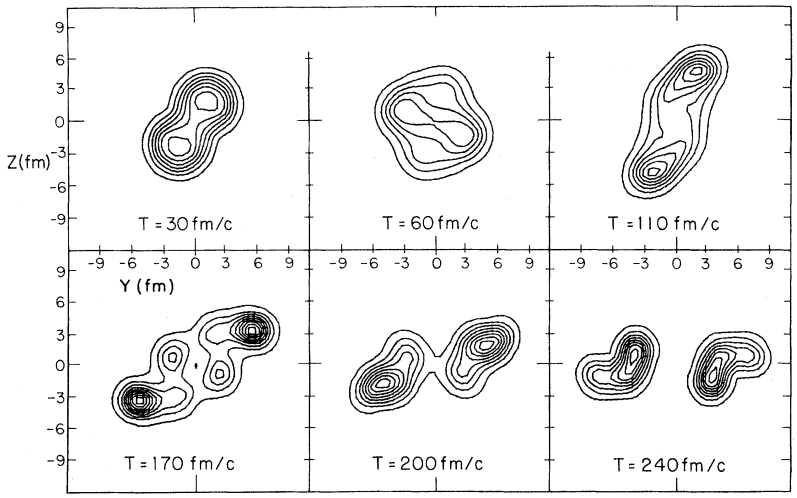

FIG. 2. Constant-value contours of the integrated density $\rho^I(y,z) = \int dx\, \rho(x,y,z)$ at various times into the reaction $^{16}O + ^{16}O$ at $E_l/A_p = 24$ MeV, $b = 4$ fm. The y-z plane is the scattering plane. At $t = (30\text{ fm})/c$ the lower fragment is moving towards the upper left-hand corner. At $t = (60\text{fm})/c$ the high-density bump near $(y,z) = (-3,+1)$ is moving towards the upper right-hand corner, while the lesser bump at $(y,z) = (1,3)$ is nearly stationary.

$\hbar\omega$(quad) are the same. This is not the case at the beginning of the collision, as expected, and furthermore, appears to be valid only once the fragments are well separated. Thus we see that the multifluid process described above appears to invalidate a meaningful description in terms of a rigid rotation with a rigid moment of inertia. The collective energy versus time is also shown in Fig. 1. The small fluctuations superimposed on the general behavior represent high-order multipole collective motion which persists as complex nonaxial internal oscillations of the fragments as they come apart. These oscillations can be observed in Fig. 2 at $t = (110,\ 170,\ \text{and}\ 200\text{ fm})/c$. It is perhaps not too surprising to note that the isolated bumps which appear near $t = (170\text{ fm})/c$ have a size similar to that of an α particle. Further calculations including Coulomb and evaporation effects will be reported later. In conclusion, we see that the three-dimensional TDHF method appears capable of a rich and varied description of heavy-ion reactions, while it appears not to support the simplified rigid clutching and axiality assumptions currently applied[4] to reduce the problem to a simpler two-dimensional one.

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