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Classical microscopic description of particle cluster collisions: application to heavy ion collisions

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Abstract. A classical microscopic description of the collision between two bound particle clusters, interacting via a suitable two body force is presented with a view to extend the analogy to nuclear collisions. It is shown that with a proper choice of the parameters of the two body force, the model calculations can bring out qualitatively all the essential features of low energy heavy ion collisions such as complete fusion, deep inelastic scattering and nucleon transfers. The model avoids some of the limitations of purely hydrodynamic descriptions connected with the shape parametrization, compressibility and viscosity effects, etc.

Keywords. Heavy ion collisions; fusion; deep inelastic scattering; nucleon transfer; classical microscopic description; Lennard-Jones potential.

1. Introduction

In studying the dynamics of heavy ion collisions, one may use either a microscopic approach (Koonin 1976; Bonche *et al* 1976) or a macroscopic approach (Alonso 1974). While microscopic calculations based on simple effective interactions between nucleons and quantum mechanical equations of motion are at present quite promising, their full realization still requires several extensions. On the other hand, the macroscopic approach based on the assumption of a continuous distribution of nuclear matter subjected to given forces, has been very widely used in the study of fission and heavy ion fusion dynamics, both because of its relative conceptual simplicity and ease of numerically solving the relevant equations of motion. Irrespective of the precise approach that is taken, a problem of central importance is the large scale transfer of energy from relative motion to internal excitation of the colliding nuclei. While in a purely microscopic calculation, this is determined automatically through the solution of the time-dependent many body equations, in a macroscopic approach, one has to consider separately the collective degrees of freedom which describe the overall macroscopic properties of the nuclei such as the shape and their internal degrees of freedom describing the motion of the nucleons and invoke a suitable mechanism for the transfer of energy from the collective to the internal degrees. As of today, it is not even clear whether the basic mechanism for this transfer of energy is by means of individual two body collisons as in the case of ordinary fluids (Swiatecki 1972) or by means of nucleons colliding with a moving potential wall (Swiatecki 1975). In order to decide between these two alternatives, calculations based on both these mechanisms of energy transfer are being carried out.

While these calculations have led to much insight into various aspects of nuclear collective dynamics particularly with regard to the dynamics of fissioning nuclei, in the field of heavy ion fusion and scattering, some inherent inadequacies of these calculations have been recognized. Firstly, the idealization of a nucleus as a charged liquid drop with continuous distribution of nuclear matter and a sharp surface as the relevant collective degree of freedom, while being a reasonably good approximation in and near equilibrium configurations, becomes questionable for highly deformed nuclear shapes encountered in fission and heavy ion fusion, particularly in those regions of deformations where the local radii of curvature become comparable to the surface diffuseness of the nuclear surface (or the range of nuclear force). Secondly, even the choice of a suitable parametrization of the nuclear shape, capable of describing all the possible relevant shapes is still in an unsatisfactory stage.

Another simple approach which has been recently investigated is the classical microscopic approach (Bodmer and Panos 1977; Bondorf *et al* 1976; Wilets *et al* 1977). In this approach, the nucleons in the colliding nuclei are taken as classical spinless particles interacting via a suitable two body force. In a collision, the trajectories of all the nucleons are computed on the basis of classical non-relativistic equations of motion and the forces between all pairs of nucleons. This approach, similar to the molecular dynamics description of liquids (Rahman 1964) avoids some of the limitations of the purely hydrodynamical approach, and at the same time includes hydrodynamics as a limit. Since all the translational degrees of the constituent nucleons are explicitly included in the calculations, there is no need to separate the dynamics of the collective degrees of freedom from the intrinsic degrees. All dissipation and transfer of energy arise due to nucleon-nucleon collisions and are built-in in the calculations. It has been argued (Bodmer and Panos 1977) that for laboratory energies of a few hundred MeV per nucleon or more, classical considerations may be expected to be reasonably good and hence these calculations have been restricted to high energy nuclear collisions only. In the present work, we describe a classical trajectory calculation in the collision between two bound particle clusters interacting via suitable two body forces. It is shown on the basis of an analysis of the collision trajectories that the collisions exhibit qualitatively all the essential features of low energy heavy ion collisions also such as complete fusion, deep inelastic scattering and nucleon transfer.

2. Description of the model

The central input to the model is the two body force. Having chosen a suitable two body potential and therefore the corresponding force between any pair of particles, the classical trajectories of any system of particles for a given set of initial conditions can be obtained by numerically integrating the Newton's equations of motion.

$$M\frac{d^2\bar{r}_i}{dt^2} = -\nabla_i\left(\sum_{j\neq i} V_{ij}\right)$$

where M is the mass of a particle.

For given collision conditions specified by the number of particles in each cluster, the impact parameter and the bombarding energy, the inital conditions correspond to the initial distribution of particle positions in each cluster, and a uniform velocity for all particles in each cluster. The particle trajectories thus computed can be used to study any desired macroscopic feature of the collision.

2.1. *Choice of the particle-particle potential*

Keeping in view the application of the present calculations to heavy-ion collisions, a tempting choice of the particle-particle potential is the free nucleon-nucleon potential suitably averaged over the possible angular momentum states. However, this potential without an explicit inclusion of the uncertainty principle and the resulting zero point motion leads to particle clusters which have too large binding energy per particle and too large particle density in their stable ground state. Efforts to include the zero point motion in these calculations are still in a rudimentary stage and are far from satisfactory. For instance, the frequently used technique of arbitrarily assigning finite kinetic energies to the particles, leads to an unavoidable premature evaporation of the particles during the interaction time. Another possible approach in the choice of the inter-particle potential is to adopt a purely phenomenological form for the potential, with the constants so chosen as to ensure that the equilibrium macroscopic properties of the particle clusters in their stable ground state are close to those of nuclei. The calculation, while being fully classical are internally self consistent, and the model is analogous to the liquid drop model of the nucleus. Further, it is a microscopic description of the nucleus free from continuum approximations of the LDM. This is the approach that we have adopted in the present calculations. While the choice of such a phenomenological potential is not expected to be unique, we have taken guidance from the molecular dynamics calculations for classical liquids and choose a Lennard-Jones form for the particle-particle potential. Thus the potential between any pair of particles is

$$V(r_{ij}) = \epsilon\,[(\sigma/r_{ij})^{12} - 2(\sigma/r_{ij})^{6}]$$

Figure 1 shows a plot of the potential in units of ϵ as a function of the inter-particle distance r in units of σ. For such an interaction potential, minimum energy configurations as a function of particle number have been studied earlier (Hoare and Pal 1971). Figure 2 shows a plot of binding energy per particle as a function of $N^{-1/3}$. It is seen that a linear relation of the form $\bar{B}E/N=a_0-a_1 N^{-1/3}$ holds for $10<N<60$. Therefore, it can be concluded that a Lennard-Jones form for the interaction potential is a good approximation even for ' nuclear droplets ' as far as their macroscopic properties are concerned. We have, therefore, adopted the above Lennard-Jones form for particle-particle interaction potential. In addition, in analogy with nuclei some of the particles are assumed to be charged and an usual Coulomb term is added to the interaction potential. Also the potential between like particles was taken to be about 20% weaker than that between unlike particles (Myers and Swiatecki 1969). (A Lennard-Jones fluid, however, has a compressibility coefficient larger than that of nuclei. In this sense, the present model is closer to an incompressible liquid drop).

With this choice of the two body potential the equilibrium spatial distributions of the particles in any cluster can be obtained as follows: A random distribution of all the A particle positions is generated in a cube of side $2R$, where R is approximately the size of the cluster. This random distribution of particle positions is in general energetically very unfavourable. With the initial particle velocities equal to zero, this distribution is allowed to dynamically evolve following classical equations of motion. However, the particle velocities are set equal to zero at the end of each time step so that the initial velocities are zero for the succeeding interval. At each step,

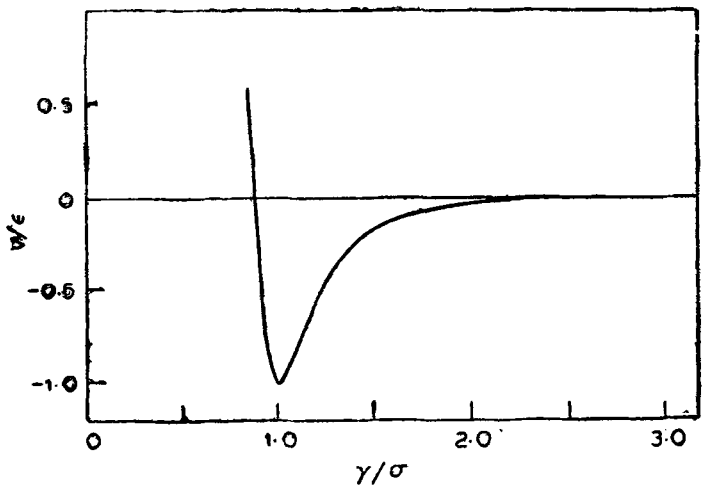

Figure 1. The Lennard-Jones potential $V(r) = \epsilon[(\sigma/r)^{12} - 2(\sigma/r)^6]$.

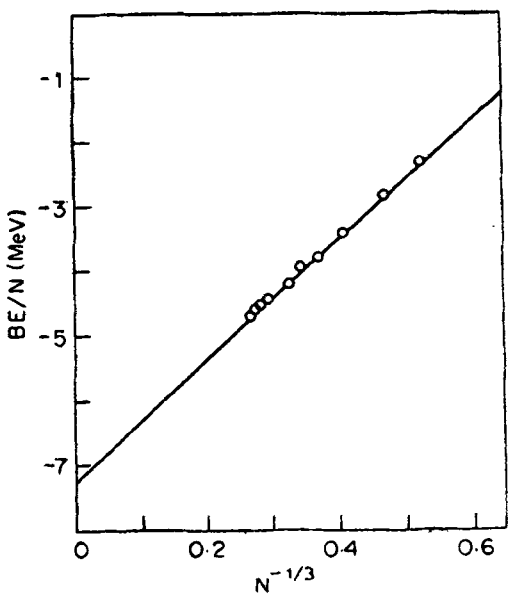

Figure 2. Plot of the binding energy per particle versus $N^{-1/3}$ for one component clusters.

various macroscopic properties of the assembly of particles such as the size, the total potential energy, etc. are monitored. The calculations are continued till all these macroscopic quantities settle down to their equilibrium values. The total potential energy also acquires its minimum value at this stage. Such a minimum corresponds to a frozen system at zero temperature when the particles are arranged approximately in a lattice. The corresponding particle positions are used, as will be discussed in the next section, as the initial positions for the particles in a collision calculation. These calculations have been carried out as a function of number of particles in the clusters. The calculations were carried out for $N=Z=A/2$ clusters. Figure 3a shows a plot of the binding energy per particle ($\equiv 1/2A\ \Sigma_{ij}\ V_{ij}$ evaluated for the equilibrium configuration) without the Coulomb part in units of ϵ versus $A^{-1/3}$ and figure 3b shows the root mean square radii ($\equiv [(\bar{r}_i-\bar{R})^2]^{1/2}$ where $\bar{R}$ is the position of the centre of mass of the cluster) in units of σ versus $A^{1/3}$. Again, it is seen that both the binding energy per particle and the r.m.s. radii exhibit a linear dependence on $A^{-1/3}$ and $A^{1/3}$ respectively. With a choice of $\epsilon = 2{\cdot}2$ MeV and $\sigma = 1{\cdot}8$ fm, the macroscopic properties of these clusters are close to the liquid drop model values of nuclei with a mean binding energy per particle of 16 MeV in the interior of the nucleus and a radius $1{\cdot}2\ A^{1/3}$ fm.

2.2. *Specification of initial conditions and the calculation of collision trajectories*

The present calculations have been carried out for $A_1=A_2=16$ with half the particles charged in each cluster. The two colliding clusters were initially placed in ground state at a centre of mass distance of 20 fm where only Coulomb interaction between the clusters is effective. The distribution of particle positions in each cluster around the respective centres of mass is obtained from the energy minimization program described earlier. However, since the energy minimization leaves a continuous de-

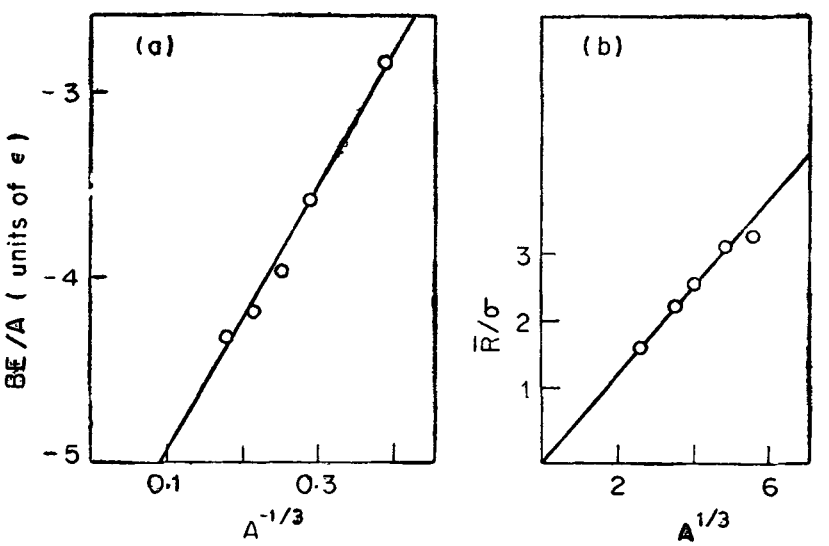

Figure 3. a. Plot of the binding energy per particle versus $A^{-1/3}$ for a two component system with equal number of particles of either species. **b.** Plot of the root mean square radius versus $A^{1/3}$ for the same systems as in *a*.

generacy with respect to the orientation of the clusters in space, arbitrary rigid rotations in space are equivalent. It is therefore necessary to repeat the calculations for various initial conditions generated by rigid rotations of the clusters and average the collision trajectories. The impact parameter and the bombarding energy further specify the magnitude and the direction of the velocities of the two clusters and therefore of the individual particles in the clusters. For a numerical solution of the equations of motion, each second order differential equation was split into two first order equations and were integrated using the standard fourth order Runga-Kutta method (Kuo 1972). Small integration time steps are to be chosen so as to ensure adequate conservation of momentum angular momentum and total energy at the same time keeping to reasonable computing times. A time step of the order of $2\text{–}5\times10^{-24}$ sec was found satisfactory in the present calculations. For distance $d > 10$ fm between the centres of mass of the two clusters the trajectories of individual clusters are Rutherford trajectories. For distances $d < 10$ fm, the trajectory can display two qualitatively different characteristics. Firstly, the energy loss from relative motion may be so large that the nuclei fuse together leading to the formation of a compound nucleus. In this case a plot of the relative distance between the centre of mass of the two clusters as a function of time will be bounded. Alternatively, after having formed a short-lived intermediate complex at small d, the system can split again into two clusters not necessarily identical to the projectile target configuration. In this case the inter-fragment distance versus time is unbounded with d going to infinity as time t tends to infinity. And the event can be identified as an elastic or inelastic scattering with or without mass exchange. The trajectories were therefore numerically computed up to $t=10^{-20}$ sec. If in this time interval the distance d remains bounded the event was identified as leading to complete fusion. Otherwise the event was identified as scattering and the trajectories were terminated when distance $d > 25$ fm.

3. Results and discussion

The collisions were studied for different impact parameters ranging from head-on to grazing angles and at different collision energies from sub-Coulomb barrier to few times the coulomb barrier. Each trajectory typically takes approximately half an hour in BESM-6 computer. The trajectories were stored in magnetic tapes for subsequent analysis.

3.1. *Head-on collisions*

In this case, if the incident energy is greater than the Coulomb barrier the two nuclei form an excited compound nucleus. Figure 4 shows a typical collision event where the projectile energy is 128 MeV. At $t=0$, the two clusters are moving towards each other in the centre of mass frame with a velocity of 0·2 fm per ls (1 ls$\equiv10^{-21}$ sec) at a centre of mass distance of 20 fm. It is seen that in an interaction time of about 0·2 ls the fusion of the nuclei is complete leading to an excited and nearly spherical system. Figure 5 shows the plot of relative kinetic energy of the two clusters as a function of time. The clusters come to a grinding halt, in a time of the order of 0·1 ls giving rise to a rate of loss of relative kinetic energy of the order 300 MeV per ls.

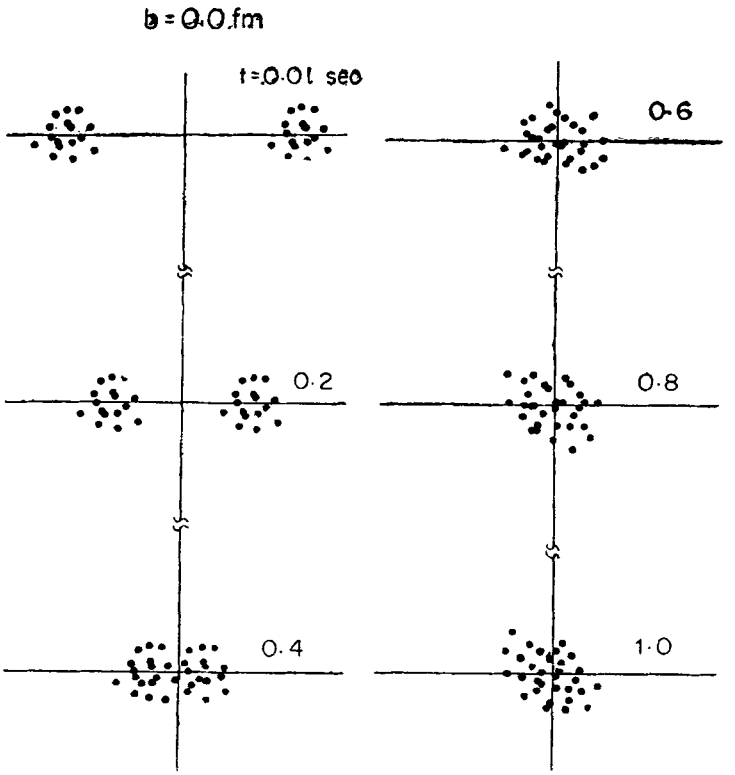

Figure 4. $X-Z$ projections of particle configurations at different times in a head-on collision event of two 16 particle clusters. The times are indicated in units of ls$=10^{-21}$sec and the collision energy is 64 MeV in the CM frame. The event leads to a complete fusion of the colliding clusters.

We have also analysed some of the macroscopic properties of the clusters in the collision process. Following Nix and Sierk (1974) two macroscopic variables were defined as

$$R = 2\overline{|z|}$$

and $$S = 2\,[\overline{|z|^2} - |\bar{z}|^2]^{\frac{1}{2}}$$

The variable R is a measure of the centre of mass separation distance d for separated clusters and is the measure of elongation for an unseparated cluster. The variable S is a measure of individual cluster deformation in the case of separate clusters. Figure 6 shows the collision trajectory in the (R, S) plane, for the case $v=0{\cdot}2$ fm per ls. Also shown in the figure, are the locii of points representing single spheroids and touching spheroids. It can be seen that the collision leads to the fusion of two colliding clusters and the resulting excited nucleus getting into a predominantly spheroidal oscillation. Also shown in the figure for comparison is the collision trajectory for the sub-barrier case, where the colliding clusters are scattered back. It is interesting to note that the trajectory in the entrance and the exit channels are not the same.

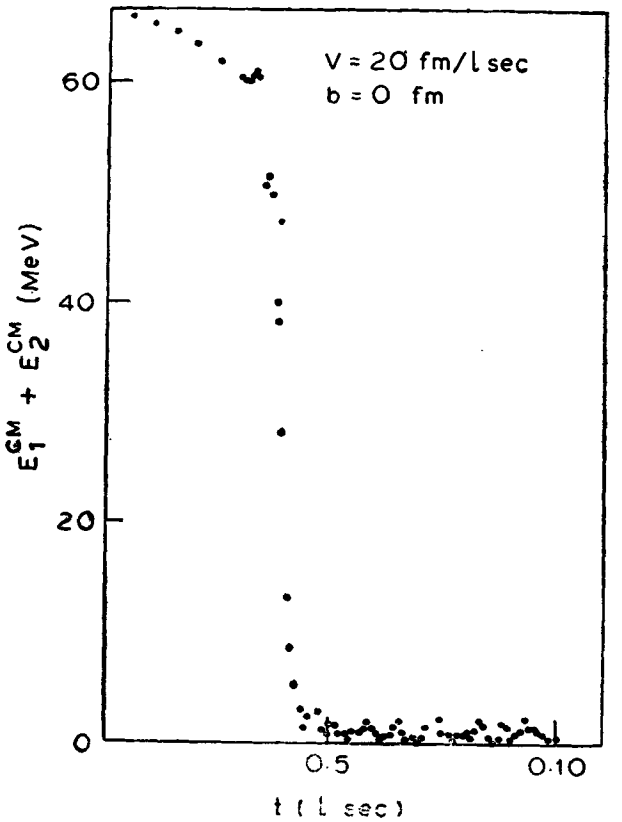

Figure 5. Plot of the kinetic energy in relative motion as a function of time for the same head-on collision event shown in figure 4.

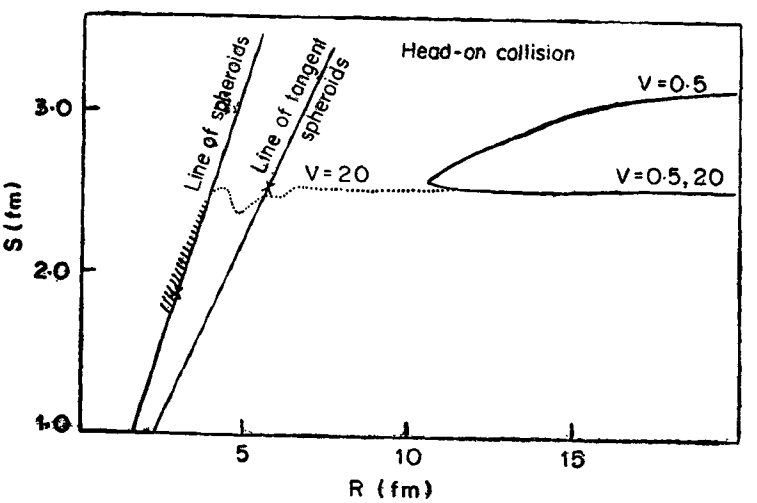

Figure 6. Typical collision trajectories in the $(R-S)$ plane for two head-on collision events. The macroscopic coordinates R and S are defined in the text. The event with CM velocity 20 fm/ls leads to complete fusion of the colliding clusters whereas the event with 5 fm/ls has a collision energy below the Coulomb barrier and leads to scattering of the clusters but in a different exit channel.

While the two clusters almost retain their spherical shape in the entrance channel, they go over to prolate deformed shapes in the exit channel. This observation amply justifies the often made assumption that the entrance and exit channel deformations are not the same (Wilczynska and Wilczynski 1976; De *et al* 1976).

3.2. *Peripheral collisions*

We now give some typical results of collisions with non-zero impact parameters b. In these calculations the collision energy was kept fixed at 128 MeV. Figures 7a and

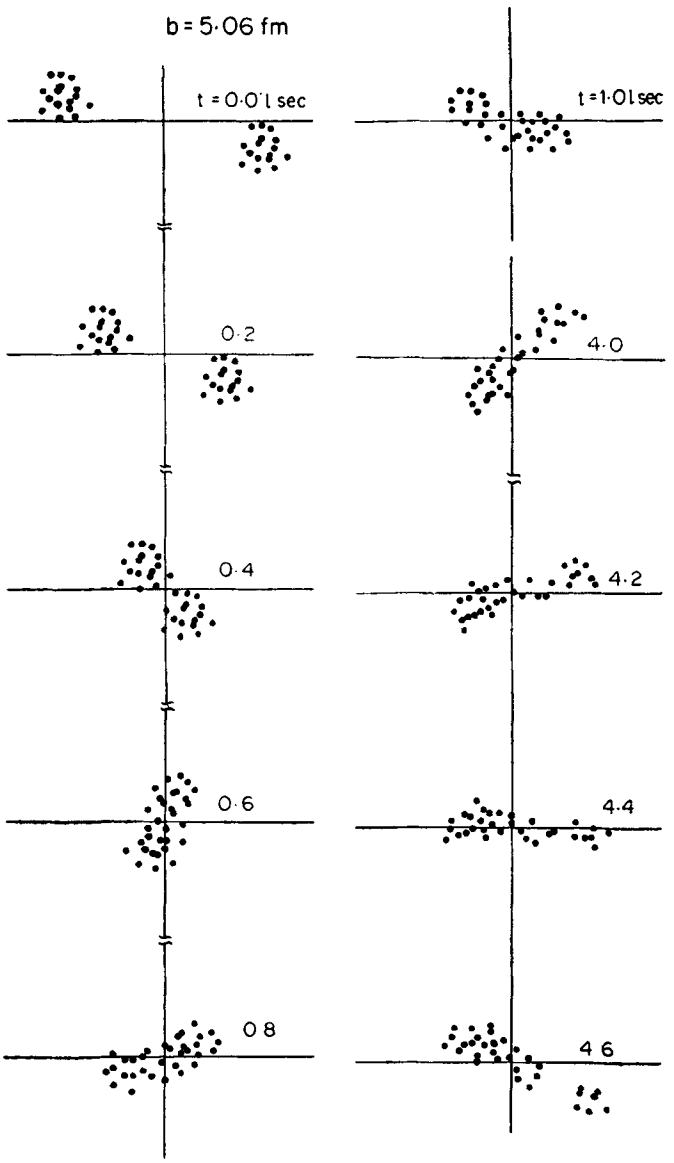

Figure 7a. Same as figure 4 for peripheral collisions. Impact parameter $b = 5{\cdot}06$ fm;

7b show two trajectories for impact parameters $b=5{\cdot}1$ fm and $b=5{\cdot}06$ fm. Essentially the trajectories demonstrate the formation of a rotating intermediate complex which subsequently separates into two clusters with or without particle exchange. For impact parameters $b<5{\cdot}0$ fm, the clusters fuse together completely. And for impact parameters $b>6{\cdot}0$ fm, the scattering is almost elastic. In the intermediate impact parameter $5<b<6$ fm, deep-inelastic scattering occurs. Figure 8 shows the trajectory of the centre of mass of one of the fragments for various b values. Table 1 lists the asymptotic centre of mass kinetic energy of the pair clusters, their scattering angle and the mass ratio for the different cases, and it can be seen from figures 7 and 8 that with decreasing impact parameters there is a monotonic increase in the life time of the intermediate complex, the energy loss from relative motion and the number of particles exchanged. The rate of energy loss from relative motion was found to be

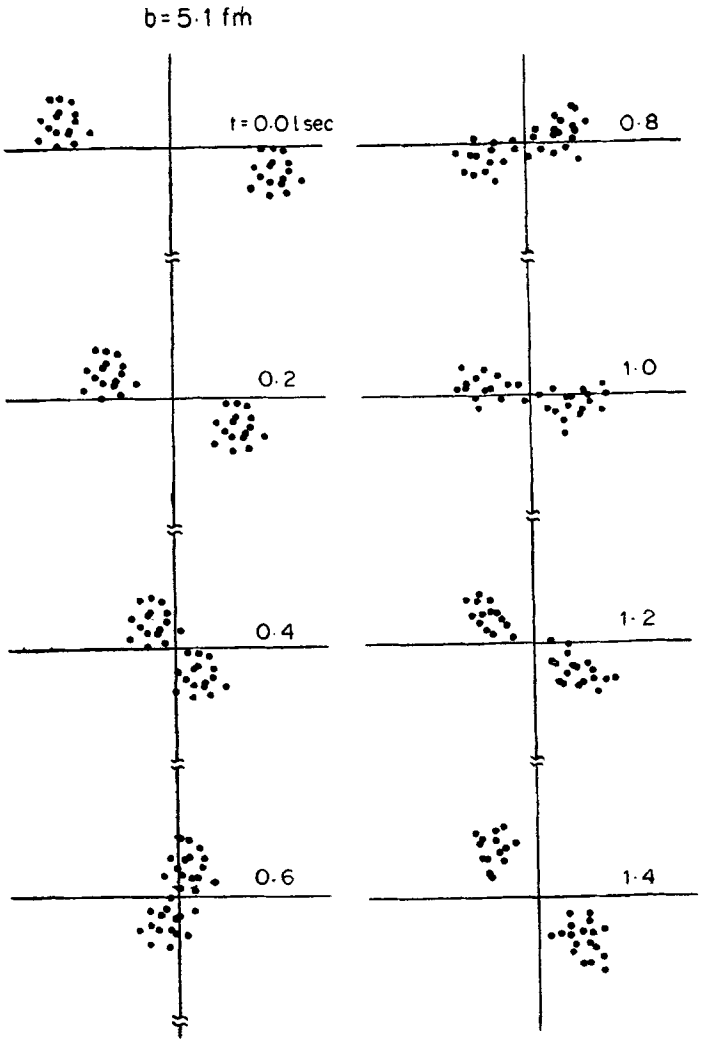

Figure 7b. Same as figure 4 for peripheral collisions. Impact parameter $b=5{\cdot}1$ fm.

of the order of 200–300 MeV/ls. These observations are qualitatively in good agreement with the experimentally well known features of the deep inelastic reactions in heavy ion collisions (Schroder and Huizenga 1977).

Table 1. Entrance and asymptotic exit channel parameters for the different collision events (i) to (vi) shown in figure 8.

	b fm	E_F^{CM} MeV	$A_1^F - A_2^F$	Life time ls
i	7·0	66·6	0	0
ii	6·0	53·0	0	0·1
iii	5·2	24·0	2	0·3
iv	5·1	12·0	2	0·8
v	5·06	10·2	6	1·4
vi	5·0	10·0	18	5·5

b = impact parameter
E_F^{CM} = Kinetic energy in relative motion of the separating clusters
$A_1^F - A_2^F$ = Mass difference between the separating clusters
l = Life-time of the intermediate rotating complex

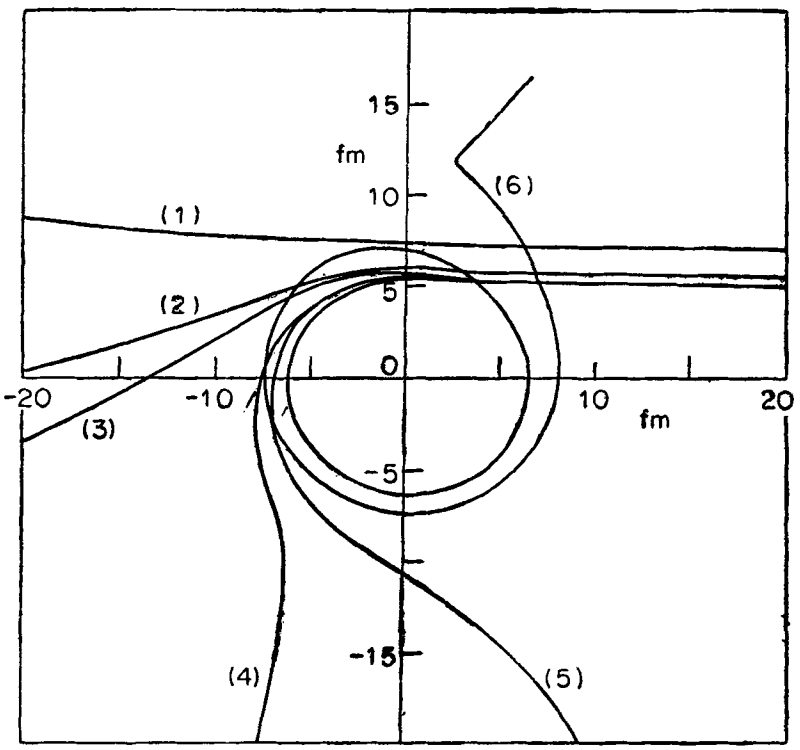

Figure 8. Centre of mass trajectories of one of the colliding clusters for cases with different impact parameters. The CM collision energy is 68 MeV in all the cases. The entrance and the asymptotic exit channel parameters for the different cases (i) to (vi) are given in table 1.

Keeping in mind our *a priori* knowledge that a classical description is inadequate to describe the detailed motions of nucleons in nuclei, these results are somewhat surprising. The model perhaps owes its success to the possibility that the above features of low energy heavy ion collisions are essentially classical in origin and quantum effects play only a perturbing role. In this case, it is likely that the present calculation can serve as a good starting point for a more vigorous semiclassical description. Alternately, the model is equivalent to a hydrodynamic description with finite meshes, where the system is split into a finite number of mass points for numerical solution. The particle-particle potential in the present case is only a different representation of the hydrodynamical equation of state but with no internal structure of the mass points. We prefer the former viewpoint.

4. Conclusions

Taking guidance from molecular dynamics description of classical liquids, we have studied the dynamics of collision of two bound particle clusters starting from a simple particle-particle potential and classical equations of motion. The potential chosen is of the Lennard-Jones form and with a suitable choice of the parameters, the macroscopic properties of the clusters in their ground state resemble those of incompressible liquid drop model nuclei. The collision dynamics is studied by computing the individual trajectories of all the particles numerically for different initial conditions such as collision energy and impact parameters. It is shown that the model brings out most of the essential features of heavy ion collisions such as complete fusion, deep inelastic scattering and particle exchange. The present model calculations, while being classical, do not involve some of the inadequacies of the conventional liquid drop model such as shape parametrization, viscosity effects, etc. We believe that these calculations can not only provide important guidelines for a macroscopic description as in the selection of relevant degrees of freedom but can also serve as a good starting point for a semiclassical microscopic description.

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