Dynamical and Statistical Modelling of Many Body Collisions Part I: Scattering

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Abstract. Although rarefied gas dynamics has traditionally rested on the dilute gas assumption, which presupposes that only binary collisions and single-body gas surface interactions occur, expressions for many-body collision rates and for many-body gas surface interaction (GSI) rates seem to suggest that at lesser heights the dilute gas assumption is not valid. In particular, in the pure rarefied regime, two-body GSIs and some three-body interactions occur whereas, in the transition regime into continuum flow, four body collisions and four body GSIs occur. In this paper I formulate many body collisions using dynamical and statistical modelling. I show that the results of binary collisions can be useful in formulating many body collisions. In particular, I show that the equations of motion of a many body system can be recast into the equations of motion of a number of reduced particles which scatter in space as well as exchange energy with one another and with the centre of mass of the system. For \(N\)-interacting bodies there are \(N-1\) reduced particles. In this paper I focus on the scattering of the reduced particles. For two-body collisions the scattering of the single reduced particle is confined to a single plane. However, for many body collisions the equations of motion show that the scattering of each reduced particle occurs in space. Hence, there is an in-plane deflection as well as an out-of-plane deflection. I calculate each deflection using the two-body formula, but with important modifications to account for the resolution of the intermolecular potential into in-plane and out-of-plane components. The magnitude of the potential is also adjusted to take account of coefficients derived from the equations of motion. I also propose an approximate model, which computes the in-plane deflection as in binary collisions but computes the out-of-plane deflection using a statistical model based on reciprocity or detailed balance. The models are designed for Direct Simulation Monte Carlo computations of rarefied gas phenomena.

I. INTRODUCTION

Many body collisions have a number of important applications in gas dynamics and astronomy. In gas dynamics, dissociation-recombination reactions occur as three-body processes. Furthermore, as the density of a gas increases from rarefied flow to continuum flow (Figure 1, Ref. 1) the frequencies of three-body and four-body collisions increase. In a high-density gas, many body collisions predominate. Dilute gases contain mainly two-body collisions, but some three-body collisions occur especially where dissociation-recombination reactions occur. In the transition region between rarefied and continuum flow, three-body and four-body collisions predominate – with a few two-body collisions occurring. However, in continuum flow (high-density gases) the closeness of the molecules means that four-body, five-body and even higher order collisions predominate. In spite of this importance of many body collisions not much research has gone into its investigation. This is because its significance has not been previously recognised. Moreover, many body problems are particularly difficult in view of their dynamical intractability.

In this article I describe a breakthrough which allows complete solution of many-body problems, which have remained intractable on purely dynamical considerations. The breakthrough lies in combining dynamical and statistical principles. The philosophy is to solve dynamically whatever part of the problem we can solve using dynamical techniques, and to solve statistically whatever part of the problem we cannot solve using dynamical techniques. In applying dynamics to the problem we draw inspiration from well-known two body results. In particular, a binary collision can be reduced to the central force motion of a reduced particle which interacts with a fixed centre of force within a fixed collision plane. I show that many body collisions can be reduced to the central force motion of a
number of reduced particles, each of which interacts with a fixed centre of force in three-dimensional space. The motion is not confined to a fixed collision plane. Instead the incident plane is deflected into a post-collision plane through the interaction. A reduced particle is formed between a reference particle and any of the other particles. I show that each reduced particle suffers a primary in-plane deflection in addition to secondary deflections caused by the other particles. These other particles also cause out-of-plane deflections which manifest as a deflection of the incident plane into a post-collision plane. I calculate these deflections by extending the well-known two-body deflection formula.

To find the post-collision speeds of the reduced particles I use conservation of energy and invoke a statistical formulation based on reciprocity or detailed balance. This approach introduces a single model parameter which can be obtained from the temperature dependence of the transport properties of gases. Knowing the angles of deflection and post-collision speeds of each reduced particle we can calculate the post-collision velocities of the interacting bodies.

I illustrate the general principles using three- and four-body encounters and then I generalise to N-bodies wherever possible. However, the same basic principles can be applied to any number of interacting bodies. You simply get more reduced particles, more secondary contributions to the in-plane deflection of each reduced particle and more contributions to the out-of-plane deflection of each reduced particle. The energy exchange calculation simply accounts for more reduced particles, but still remains tractable. However, the final transformation model for the energy exchange becomes ever more complex. This approach develops models that can be used in the Direct Simulation Monte Carlo (DSMC) method, which is the standard method of computing rarefied gas flows.

II. TWO BODY COLLISION THEORY

In a binary collision the collision plane maintains a constant orientation throughout. This means that the angular momentum vector always points in the same direction. The relative speed is also unchanged in the collision; therefore, the only effect of the collision is to deflect the initial relative velocity through an angle \( \theta \) in the collision plane.

By applying angular momentum conservation and energy conservation to the collision we can derive an expression for the deflection angle as (Ref. 2):

\[ \theta = p - 2b \int_{r_m}^{\infty} \left( 1 - \frac{b^2}{r^2} - \frac{V(r)}{2m g r^2} \right)^{\frac{3}{2}} dr \]

where: \( b = \) impact parameter, \( r = \) intermolecular separation, \( r_m = \) separation at point of closest approach, \( m = \) reduced mass of the particles, \( g' = \) relative speed, \( V = \) intermolecular potential

III. THE PHYSICS OF MANY BODY COLLISIONS

Consider the three-body problem, which is shown in Figure 1. Denote the position vector of a particle by \( \mathbf{r} \) and the intermolecular force by \( \mathbf{F} \). By writing down and manipulating the equations of motion for each particle we can re-express these equations in terms of the motion of the centre of mass as well as of two reduced particles, as follows:

\[
\begin{align*}
\dot{m_1}\mathbf{v}_{10} + m_1\mathbf{v}_{1} + m_2\mathbf{v}_{2} &= (m_0 + m_1 + m_2)\mathbf{\ddot{R}} = (m_0 + m_1 + m_2)\mathbf{\ddot{G}} = 0 \\
m_{01}\mathbf{\ddot{v}}_{01} &= -F_{01} - \frac{m_1 F_{02}}{m_0} + \frac{m_1 F_{12}}{m_1}, \quad m_{02}\mathbf{\ddot{v}}_{02} = -F_{02} - \frac{m_2 F_{01}}{m_0} - \frac{m_2 F_{12}}{m_2}
\end{align*}
\]

where \( \mathbf{R} \) and \( \mathbf{G} \) are the position and velocity of the centre of mass, and:

\[
\begin{align*}
\mathbf{r}_{01} &= \mathbf{r}_1 - \mathbf{r}_0, & \frac{1}{m_{01}} &= \frac{1}{m_0} + \frac{1}{m_1} \quad \text{or} \quad m_{01} = \frac{m_0 m_1}{m_0 + m_1}, \\
\mathbf{r}_{02} &= \mathbf{r}_2 - \mathbf{r}_0, & \frac{1}{m_{02}} &= \frac{1}{m_0} + \frac{1}{m_2} \quad \text{or} \quad m_{02} = \frac{m_0 m_2}{m_0 + m_2}
\end{align*}
\]
This result shows that the centre of mass of the three-body system travels in a straight line with constant velocity. In fact, this result applies generally for any number of interacting particles as long as the particles are not subjected to an external force.

Under an external force the centre of mass will accelerate through the collision. If the external force is denoted $F_e$ and the mean duration of a collision is $t_c$, then the post-collision velocity of the centre of mass is:

$$G' = G' + \frac{F_e}{M}dt = \frac{G'}{M} + \frac{F_e}{M}t_c$$

if $F_e$ is constant

where $M$ is the total mass of the system, i.e. the sum of the masses of the bodies making up the system.

Compared with the binary system we find that there are two extra force terms associated with the presence of the third particle. These extra force terms can be resolved into in-plane and out-of-plane components. The in-plane component further breaks down into in-line and transverse components. The in-plane component acts between the two particles used to construct the reduced particle. The transverse component acts perpendicularly to the in-line direction. The out-of-plane component acts perpendicularly to the initial collision plane. The in-line and transverse forces and separations are shown in Figures 1(b) and 3(c), in which the in-line direction is denoted $x$ and the transverse direction is denoted $y$. The effect of in-plane force components is to cause secondary in-plane deflections of the reduced particle through the collision. The primary in-plane deflection results from the primary force between the particles used to construct the reduced particle. Out-of-plane force components cause out-of-plane deflections of the reduced particle. These in-plane and out-of-plane forces combine to cause three-dimensional motion of the reduced particle through the collision.

The four-body problem is also illustrated in Figure 1(a). It can be analysed in a similar way to the three-body collision, with similar conclusions. The reduced equations of motion are:

$$m_0 \dot{r}_0 + m_1 \dot{r}_1 + m_2 \dot{r}_2 + m_3 \dot{r}_3 = (m_0 + m_1 + m_2 + m_3) \ddot{R} = (m_0 + m_1 + m_2 + m_3) \ddot{G} = 0$$

$$m_{12} \ddot{r}_{12} = -F_{01} - \frac{m_1}{m_{12}} (F_{02} + F_{03}) - \frac{m_2}{m_{12}} (F_{12} + F_{13})$$

$$m_{23} \ddot{r}_{23} = -F_{03} - \frac{m_3}{m_{03}} (F_{01} + F_{02}) - \frac{m_2}{m_{13}} (F_{13} + F_{23})$$

where: $r_{03} = r_3 - r_0$, $\frac{1}{m_{03}} = \frac{1}{m_0} + \frac{1}{m_3}$ or $m_{03} = \frac{m_0 m_3}{m_0 + m_3}$

Apart from indicating the extra forces that act on a reduced particle, and that make it depart from the two-body collisions, note that the equation of motion for each reduced particle also indicates the proportion and sign of each extra force that affects the motion of a reduced particle. The proportions and signs are indicated by the coefficients of the forces that appear on the RHS of the equation of motion for each reduced particle. Note that we must multiply the potential function used to represent each force, in the deflection angle formula, by the correct coefficient and sign for each force. A negative force implies a positive potential and vice versa. We shall use these findings below to formulate deflection angle formulae. Note finally that the foregoing principles can be applied to any number of interacting bodies.

### IV. RESOLVING POTENTIALS AND SEPARATIONS

In formulating deflection angle formulae we find that we have to resolve a potential function into in-plane and out-of-plane directions. ‘In-plane’ means in the collision plane and ‘out-of-plane’ means in the normal direction to the collision plane. Since the collision plane changes through the interaction we use the initial collision plane as our reference collision plane. There are two in-plane directions: in-line and transverse. The in-line direction is along the intermolecular separation of the two particles that are used to form the reduced particle whose motion is being considered. The transverse direction is normal to this. Whereas the in-plane potential induces in-plane deflections the out-of-plane potential induces out-of-plane deflections. The original potential is assumed to depend only on $r$, where this is the intermolecular separation between one of the two particles lying in the in-line direction and some other particle of the system. We assume that the in-line direction is $x$, the transverse in-plane direction is $y$, and the out-of-plane direction is $z$. Thus $x$ and $y$ lie in the initial collision plane whereas $z$ lies perpendicular to this plane. Note that
(x, y, z) is thus used to denote either the separations or the position co-ordinates of the particles. No conflict arises as long as the context is kept in mind.

Given the original potential:

\[ V = V(r), \text{ where } r^2 = x^2 + y^2 + z^2, \text{ such that } F_r = -\frac{\partial V(r)}{\partial r} \]

we want to resolve the potential along x, y, and z, such that:

\[ F_x = -\frac{\partial V(r)}{\partial x}, \quad F_y = -\frac{\partial V(r)}{\partial y}, \quad F_z = -\frac{\partial V(r)}{\partial z} \]

where \( \mathbf{F} = (F_x, F_y, F_z) \) is the force generated by \( V \).

Knowing that:

\[ F_x = -\frac{x}{r} \frac{dV(r)}{dr}, \quad F_y = -\frac{y}{r} \frac{dV(r)}{dr}, \quad F_z = -\frac{z}{r} \frac{dV(r)}{dr} \]

we get:

\[ V_x = \int_0^x \frac{dV(r)}{dr} \, dx, \quad V_y = \int_0^y \frac{dV(r)}{dr} \, dy, \quad V_z = \int_0^z \frac{dV(r)}{dr} \, dz \]

If we assume that along x we have y = 0, z = 0; along y we have x = 0, z = 0; and along z we have x = 0, y = 0 then the preceding relations simplify to:

\[ V_x = V(x), \quad V_y = V(y), \quad V_z = V(z) \]

Note that the potentials depend only on distances, not directions. This means that the potentials are spherically symmetric.

To resolve separations and other vectors along the three orthogonal directions we need the unit vectors along these directions. For the in-line direction we can use the separation vector along that direction to construct the unit vector. For the out-of-plane direction we use the angular momentum vector to construct the unit vector. Cross-multiplying these unit vectors gives the unit vector in the transverse in-plane direction. The results are:

In-line : \( \frac{r_0}{r_0} \), Out-of-plane : \( \frac{r_0 \times g_j}{|r_0 \times g_j|} \), Transverse : \( \frac{r_0 \times g_j}{|r_0 \times g_j|} \)

**V. DEFLECTION ANGLE CALCULATION**

The primary and secondary deflection angles have the general form:

\[ c_{jk} \text{ (or } e_{jk} \text{)} = \rho - 2b \int_0^\infty \frac{dp}{p^2} \left( 1 - \frac{b^2}{p^2} - \frac{l V(p)}{2 m g^2} \right) \]

where \( l \) is the signed coefficient of the potential as given by Tables 1 and 2; and \( j,k \) are integers.

For the in-plane and out-of-plane deflection components these symbols are given appropriate meaning below.
VI. IN-PLANE DEFLECTION CALCULATION

The three dimensional central force motion of each reduced particle in a many body collision is illustrated in Figure 2 which shows the motion resolved in a vertical and a horizontal plane. In the vertical plane in-plane motion is illustrated. This is caused by in-plane forces and results in the in-plane deflection of the relative velocity through an angle \( \mathbf{c} \). In the horizontal plane we get out-of-plane motion caused by the out-of-plane forces. This manifests in a deflection of the initial plane of the collision through an azimuthal angle \( \mathbf{e} \). Similarity with the two-body geometry is clear. In fact we can apply the two-body deflection angle formula, with appropriate modifications, to the many body problem.

Taking into account the result described earlier that each of the extra forces in the dynamic equation for a reduced particle exerts only a fractional influence on the motion of the reduced particle, and that the sign of these effects are important, we can write down an expression for the in-plane and out of plane deflections. The sign and proportion for each force is extracted directly from the dynamic equation of each reduced particle. Table 1 shows the coefficients for three-body collisions whereas Table 2 shows the results for four-body collisions. Note that a positive force leads to a negative potential and vice versa. In the subsequent formulae we use the following symbols:

\[ c_{(1)} = \text{in-plane deflection angle for reduced particle } m_i \]
\[ c_{(0)} = \text{primary deflection angle, the rest being secondary} \]
\[ b_{ci} = \text{impact parameter for in-plane scattering of reduced particle } m_i \]
\[ r_{0i} = \text{intermolecular separation for reduced particle } m_i \]
\[ r_{0im} = \text{separation at point of closest approach} \]
\[ x_{jk} = \text{in-line component of } r_{jk}, \quad x_{jkm} = \text{component at point of closest approach} \]
\[ y_{jk} = \text{transverse in-plane component of } r_{jk}, \quad y_{jkm} = \text{component at point of closest approach} \]
\[ q_{jk} = \text{resultant of } x_{jk} \text{ and } y_{jk}, \quad q_{jkm} = \text{resultant at point of closest approach} \]
\[ V_{jk} = \text{intermolecular potential}, \quad V' = \text{initial relative speed for reduced particle } m_i \]

The in-plane deflection angles for three body collisions are then:

(a) First reduced particle.

\[ c_{(01)} = c_{(1)} + c_{(2)}, \quad \text{with } c_{jk} \text{ being given by (5) where the symbols are : } b = b_{c01}, \quad m = m_{01}, \quad g' = g'_{01}, \quad \text{and for } c_{01} : \quad p = r_{01}, \quad V = V_{01}, \quad l = 1; \quad \text{for } c_{02} : \quad p = q_{02}, \quad V = V_{02}, \quad l = \frac{m_{01}}{m_0}; \quad \text{for } c_{12} : \quad p = q_{12}, \quad V = V_{12}, \quad l = \frac{m_{01}}{m_i}; \]

where \( q_{jk} = \left( x_{jk}^2 + y_{jk}^2 \right)^{\frac{1}{2}}, \quad x_{jk} = r_{jk} \cdot \frac{r_{01}}{r_{01}}, \quad y_{jk} = r_{jk} \cdot \left( \frac{r_{01} \times r_{01} \times g_i}{r_{01} \times g_i} \right) \)

(b) Second reduced particle.

\[ c_{(02)} = c_{(2)} + c_{(1)}, \quad \text{with } c_{jk} \text{ being given by (5) where the symbols are : } b = b_{c02}, \quad m = m_{02}, \quad g' = g'_{02}, \quad \text{and for } c_{02} : \quad p = r_{02}, \quad V = V_{02}, \quad l = 1; \quad \text{for } c_{01} : \quad p = q_{01}, \quad V = V_{01}, \quad l = \frac{m_{02}}{m_0}; \quad \text{for } c_{12} : \quad p = q_{12}, \quad V = V_{12}, \quad l = \frac{m_{02}}{m_i}; \]

where \( q_{jk} = \left( x_{jk}^2 + y_{jk}^2 \right)^{\frac{1}{2}}, \quad x_{jk} = r_{jk} \cdot \frac{r_{02}}{r_{02}}, \quad y_{jk} = r_{jk} \cdot \left( \frac{r_{02} \times r_{02} \times g_i}{r_{02} \times g_i} \right) \)

The in-plane deflection angles for four body collisions are:
(a) First reduced particle.
\[ C_{(01)} = C_{01} + C_{02} + C_{03} + C_{12} + C_{13}, \]
with \( C_{jk} \) being given by (5) where the symbols are: \( b = b_{c01}, \ m = m_{b1}, \ g' = g'_{01}, \)
and for \( C_{01} : \ p = r_{01}, \ V = V_{01}, \ l = l_1; \) for \( C_{02} : \ p = q_{02}, \ V = V_{02}, \ l = \frac{m_{b1}}{m_0}; \) for \( C_{03} : \ p = q_{03}, \ V = V_{03}, \ l = \frac{m_{b1}}{m_0}; \) 
for \( C_{12} : \ p = q_{12}, \ V = V_{12}, \ l = -\frac{m_{b1}}{m_1}; \) for \( C_{13} : \ p = q_{13}, \ V = V_{13}, \ l = -\frac{m_{b1}}{m_1}; \)
where 
\[ q_{jk} = \left( x_{jk}^2 + y_{jk}^2 \right) \frac{r_{01}}{r_{01}}, \quad x_{jk} = \frac{r_{01} \times r_{01} \times g_1}{\left| r_{01} \times g_1 \right|}, \quad y_{jk} = \frac{r_{02} \times r_{02} \times g_2}{\left| r_{02} \times g_2 \right|}, \quad j, k \text{ being integers} \]

(b) Second reduced particle.
\[ C_{(02)} = C_{02} + C_{01} + C_{03} + C_{12} + C_{23}, \]
with \( C_{jk} \) being given by (5) where the symbols are: \( b = b_{c02}, \ m = m_{b2}, \ g' = g'_{02}, \)
and for \( C_{02} : \ p = r_{02}, \ V = V_{02}, \ l = l_1; \) for \( C_{01} : \ p = q_{01}, \ V = V_{01}, \ l = \frac{m_{b2}}{m_0}; \) for \( C_{03} : \ p = q_{03}, \ V = V_{03}, \ l = \frac{m_{b2}}{m_0}; \) 
for \( C_{12} : \ p = q_{12}, \ V = V_{12}, \ l = \frac{m_{b2}}{m_2}; \) for \( C_{23} : \ p = q_{23}, \ V = V_{23}, \ l = -\frac{m_{b2}}{m_2}; \)
where 
\[ q_{jk} = \left( x_{jk}^2 + y_{jk}^2 \right) \frac{r_{02}}{r_{02}}, \quad x_{jk} = \frac{r_{02} \times r_{02} \times g_2}{\left| r_{02} \times g_2 \right|}, \quad y_{jk} = \frac{r_{03} \times r_{03} \times g_3}{\left| r_{03} \times g_3 \right|}, \quad j, k \text{ being integers} \]

(c) Third reduced particle.
\[ C_{(03)} = C_{03} + C_{01} + C_{02} + C_{13} + C_{23}, \]
with \( C_{jk} \) being given by (5) where the symbols are: \( b = b_{c03}, \ m = m_{b3}, \ g' = g'_{03}, \)
and for \( C_{03} : \ p = r_{03}, \ V = V_{03}, \ l = l_1; \) for \( C_{01} : \ p = q_{01}, \ V = V_{01}, \ l = \frac{m_{b3}}{m_0}; \) for \( C_{02} : \ p = q_{02}, \ V = V_{02}, \ l = \frac{m_{b3}}{m_0}; \) 
for \( C_{13} : \ p = q_{13}, \ V = V_{13}, \ l = \frac{m_{b3}}{m_3}; \) for \( C_{23} : \ p = q_{23}, \ V = V_{23}, \ l = \frac{m_{b3}}{m_3}; \)
where 
\[ q_{jk} = \left( x_{jk}^2 + y_{jk}^2 \right) \frac{r_{03}}{r_{03}}, \quad x_{jk} = \frac{r_{03} \times r_{03} \times g_3}{\left| r_{03} \times g_3 \right|}, \quad y_{jk} = \frac{r_{03} \times r_{03} \times g_3}{\left| r_{03} \times g_3 \right|}, \quad j, k \text{ being integers} \]

VII. COLLISION PLANE CALCULATION: OUT-OF-PLANE DEFLECTIONS

The potential functions and their signed coefficients are given in Table 1 and Table 2. These coefficients apply for both in-plane and out-of-plane deflections. However, out-of-plane motions suffer no primary deflections so that the primary potentials in Table 1 and Table 2 can be ignored. The symbols used below are as follows:

\( e_{0i} = \text{out-of-plane deflection angle for reduced particle } m_i \)
\( e_{jk} = \text{secondary deflection angle, no primary deflections exist} \)
\( b_{0i} = \text{impact parameter for out-of-plane scattering of reduced particle } m_i \)
\( z_{jk} = \text{out-of-plane component of } r_{jk}, \quad z_{jkn} = \text{component at point of closest approach} \)
\( V = \text{intmolecular potential} \quad g'_{0i} = \text{initial relative speed for reduced particle } m_i \)

The out-of-plane deflection angles for three body collisions are:
(c) First reduced particle.
\[ \theta_{01} = \theta_{02} + \theta_{12}, \] with \( \theta_{jk} \) being given by (5) where the symbols are: \( b = b_{\theta 01}, \ m = m_{\theta 1}, \ g' = g'_{\theta 01}, \) and for \( \theta_{02}: \)
\[ p = z_{02}, \ V = V_{02}, \ l = \frac{m_1}{m_0}; \] for \( \theta_{12}: \)
\[ p = z_{12}, \ V = V_{12}, \ l = \frac{m_2}{m_1}; \] where \( z_{jk} = \mathbf{r}_{jk} \cdot \left( \frac{\mathbf{r}_{01} \times \mathbf{g}_1}{|\mathbf{r}_{01} \times \mathbf{g}_1|} \right), \] \( j,k \) being integers.

(d) Second reduced particle.
\[ \theta_{02} = \theta_{01} + \theta_{12}, \] with \( \theta_{jk} \) being given by (5) where the symbols are: \( b = b_{\theta 02}, \ m = m_{\theta 2}, \ g' = g'_{\theta 02}, \) and for \( \theta_{01} : \)
\[ p = z_{01}, \ V = V_{01}, \ l = \frac{m_2}{m_0}; \] for \( \theta_{12} : \)
\[ p = z_{12}, \ V = V_{12}, \ l = \frac{m_2}{m_1}; \] where \( z_{jk} = \mathbf{r}_{jk} \cdot \left( \frac{\mathbf{r}_{02} \times \mathbf{g}_2}{|\mathbf{r}_{02} \times \mathbf{g}_2|} \right), \] \( j,k \) being integers.

The out-of-plane deflection angles for four body collisions are:

(d) First reduced particle.
\[ \theta_{01} = \theta_{02} + \theta_{03} + \theta_{12} + \theta_{23}, \] with \( \theta_{jk} \) being given by (5) where the symbols are: \( b = b_{\theta 01}, \ m = m_{\theta 3}, \ g' = g'_{\theta 03}, \) and for \( \theta_{02} : \)
\[ p = z_{01}, \ V = V_{01}, \ l = \frac{m_3}{m_0}; \] for \( \theta_{03} : \)
\[ p = z_{03}, \ V = V_{03}, \ l = \frac{m_0}{m_0}; \] for \( \theta_{12} : \)
\[ p = z_{12}, \ V = V_{12}, \ l = \frac{m_2}{m_1}; \] for \( \theta_{23} : \)
\[ p = z_{23}, \ V = V_{23}, \ l = \frac{m_2}{m_2}; \] where \( z_{jk} = \mathbf{r}_{jk} \cdot \left( \frac{\mathbf{r}_{01} \times \mathbf{g}_1}{|\mathbf{r}_{01} \times \mathbf{g}_1|} \right), \] \( j,k \) being integers. 

(e) Second reduced particle.
\[ \theta_{02} = \theta_{01} + \theta_{03} + \theta_{12} + \theta_{23}, \] with \( \theta_{jk} \) being given by (5) where the symbols are: \( b = b_{\theta 02}, \ m = m_{\theta 3}, \ g' = g'_{\theta 03}, \) and for \( \theta_{01} : \)
\[ p = z_{01}, \ V = V_{01}, \ l = \frac{m_3}{m_0}; \] for \( \theta_{03} : \)
\[ p = z_{03}, \ V = V_{03}, \ l = \frac{m_0}{m_0}; \] for \( \theta_{12} : \)
\[ p = z_{12}, \ V = V_{12}, \ l = \frac{m_2}{m_2}; \] for \( \theta_{23} : \)
\[ p = z_{23}, \ V = V_{23}, \ l = \frac{m_2}{m_2}; \] where \( z_{jk} = \mathbf{r}_{jk} \cdot \left( \frac{\mathbf{r}_{02} \times \mathbf{g}_2}{|\mathbf{r}_{02} \times \mathbf{g}_2|} \right), \] \( j,k \) being integers.

(f) Third reduced particle.
\[ \theta_{03} = \theta_{02} + \theta_{03} + \theta_{13} + \theta_{23}, \] with \( \theta_{jk} \) being given by (5) where the symbols are: \( b = b_{\theta 03}, \ m = m_{\theta 3}, \ g' = g'_{\theta 03}, \) and for \( \theta_{02} : \)
\[ p = z_{02}, \ V = V_{02}, \ l = \frac{m_3}{m_0}; \] for \( \theta_{03} : \)
\[ p = z_{03}, \ V = V_{03}, \ l = \frac{m_0}{m_0}; \] for \( \theta_{13} : \)
\[ p = z_{13}, \ V = V_{13}, \ l = \frac{m_3}{m_3}; \] for \( \theta_{23} : \)
\[ p = z_{23}, \ V = V_{23}, \ l = \frac{m_3}{m_3}; \] where \( z_{jk} = \mathbf{r}_{jk} \cdot \left( \frac{\mathbf{r}_{03} \times \mathbf{g}_3}{|\mathbf{r}_{03} \times \mathbf{g}_3|} \right), \] \( j,k \) being integers.

VIII. AN APPROXIMATE SOLUTION

The preceding formulae constitute an exact dynamical treatment of the many body scattering. They are detailed formulae requiring a good number of integrals to be performed for the deflection angles to be obtained. We can reduce the amount of work required to compute the scattering process by reinterpretting the equations of motion of each reduced particle. We find that each equation of motion can be written in the form:
\[m_i \ddot{r}_{0i} = -F_{0i} - F_i\quad (i = 1,2,\ldots, N - 1)\]

where \(F_i\) is the resultant of all the extra forces appearing in the dynamic equation.

Compared to the two-body equation we find that the only difference is the presence of the additional force \(F_i\). As we have seen above the effect of this additional force is to cause secondary in-plane deflections and to introduce out-of-plane deflections in the reduced particle.

In determining the in-plane deflection of a reduced particle we may suppose, as a suitable first approximation, that the additional force induces no secondary in-plane deflections. Its only effect is then to induce transverse deflections. This assumption simplifies the in-plane deflection angle calculations, but becomes increasingly unrealistic as the number of interacting particles increases. The assumption implies that, as far as in-plane deflections are concerned, an \(N\) -body problem degenerates into \(N - 1\) two-body problems. The angle of deflection \(\theta_{0i}\) for each reduced particle \(\mathbf{r}_i\) is then given by the usual two-body result of equation (1).

To calculate the out-of-plane deflection we simplify the calculation by adopting certain powerful statistical ideas based on reciprocity or detailed balance. The invocation of these statistical ideas results in some loss of the physics of the collision process as embodied in a dynamical description. Nevertheless, the approach allows us to introduce an adjustable parameter which can be used to match some experimental measurement. The transformation of planes in the manner required here is identical to the transformation of planes in gas surface interactions. Therefore, we adopt a model already formulated for this process (Ref. 3). The model is:

\[f_{0i} = s_{12} f_{0i} + s_{i2} (2p - s_{i2} f_{0i}^\ast)\]

with correlation densities:

\[G_i(s') = b(s_i' | a_i, a_j) b(s_j' | a_i, 1)\quad \text{where } b(x | m, n) = \frac{1}{B(m, n)} x^{m-1} (1-x)^{n-1}, \quad (m > 0, n > 0, 0 \leq x \leq 1)\]

and \(B(m, n) = \int_0^1 x^{m-1} (1-x)^{n-1} dx\) is the beta function.

In this model, the pre-collision plane is identified by \(f\) and the post-collision plane by \(f\). The model transforms the initial plane into the final plane. The model is formulated in terms of two correlation variates – denoted by \(s\) – with densities given by two Beta distributions. The parameter \(a_i\) lies between 0 and 1 giving elastic scattering at 0 and diffuse scattering at 1.

At the lower end of the parameters we get (these results are obtained by examining the mean and variance of the first correlation variate):

\[f^\ast = f\quad \text{or scattering pattern} = d(f^\ast - f)\]

This is elastic scattering, and means that each reduced particle scatters as in binary collisions. At the upper end of the parameters we get:

\[f^\ast = 2p\quad \text{or scattering pattern} = b(f^\ast | 1, 1) = \frac{1}{2p}\]

(Note that if:

\[f\left(\frac{f^\ast}{2p}\right) = b\left(\frac{f^\ast}{2p} | 1, 1\right)\quad \text{then } f(f^\ast) = U(f^\ast | 0, 2p) = \frac{1}{2p}\]

where \(U(x | a, b) = \frac{1}{b-a}\) is the Uniform distribution with range \(a \leq x \leq b\).}

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This is the traditional diffuse scattering law; i.e. the post-collision plane is uniformly distributed between 0 and 2\(\pi\).
In particular, it is uncorrelated to the direction of the pre-collision plane. It represents an extreme case of many body effects. We expect the post-collision plane to approach this diffuse scattering law as the number of bodies increases.

## IX. ENERGY CONSIDERATIONS

The scattering behaviour of the collision determines the deflection angles for the reduced particles. We still need to determine the post-collision speeds of the reduced particles. To do so we must formulate an energy exchange between the particles. First, let us examine how to calculate the post-collision velocities in terms of the variables of the collision and then we shall examine the form of the kinetic energy in the centre of mass frame.

For the \textit{N-body problem} we obtain the post-collision velocities as:

\[
c^*_0 = G^* - \sum_{i=1}^{N-1} \frac{m_i}{M} c'_i, \quad c^*_j = G^* + \frac{M - m_j}{M} g^*_j - \sum_{i=1 \atop i \neq j}^{N-1} \frac{m_i}{M} g'_i, \quad (i, j = 1, 2, \ldots, N - 1)
\]

In the absence of external forces the centre of mass velocity is given by:

\[
G^* = G = \sum_{i=0}^{N-1} \frac{m_i}{M} c'_i = \sum_{i=0}^{N-1} \frac{m_i}{M} c_i^*
\]

In the presence of external forces the post-collision centre of mass velocity is given by (3).

To solve the collision problem completely we need to determine the post-collision relative velocities of the system. These relative velocities are the velocities of the reduced particles. We can express the relative velocities in spherical co-ordinates (Figure 3) as follows:

\[
g_{ij} = g_{ij} \sin\phi_i \cos\theta_i, \quad g_{ij}^* = g_{ij}^* \sin\phi_i \sin\theta_i, \quad g_{ij}^* = g_{ij}^* \cos\phi_i
\]

\[
g_{ij}^* = g_{ij}^* \sin\phi_i \cos\theta_i, \quad g_{ij}^* = g_{ij}^* \sin\phi_i \sin\theta_i, \quad g_{ij}^* = g_{ij}^* \cos\phi_i
\]

where \( q_i = q_i - c_i \) and \( \theta_i = \theta_i + \epsilon_i, \quad j = 1, 2, \ldots, N - 1 \)

Note that the angle \( \phi \), as used here, is the spherical polar angle, and should not be confused with the cylindrical polar angle used in the formulation of the two-particle deflection angle. Note also that a positive deflection angle leads to a decreased polar angle, as both angles increase in opposite directions. If we examine closely the results we find that all the spherical co-ordinates are determined for each reduced particle excepting the post-collision relative speeds \( g_{ij}^* \). To determine these speeds we must calculate the energy interchange among the reduced particles.

Consider first the kinetic energy in the centre of mass frame. The \textit{N-body} kinetic energy is:

\[
T = \sum_{i=0}^{N-1} \frac{1}{2} m_i c_i^2
\]

This can be expressed in the centre of mass frame in the manner (Ref. 4):

\[
T = \frac{1}{2} MG^2 + \sum_{i=0}^{N-1} \frac{1}{2} m_i (c_i - G)^2, \quad M = \sum_{i=0}^{N-1} m_i
\]

For the three-body problem this expands to:
For the four-body problem we get:

\[ T = \frac{1}{2} \frac{MG^2}{M} + \frac{1}{2} \frac{m_1 (M - m_1)}{M} s_1^2 + \frac{1}{2} \frac{m_2 (M - m_2)}{M} s_2^2 - \frac{m_1 m_2}{M} \mathbf{g}_1 \cdot \mathbf{g}_2, \quad M = m_1 + m_2 \]

For the four-body problem we get:

\[ T = \frac{1}{2} \frac{MG^2}{M} + \frac{1}{2} \frac{m_1 (M - m_1)}{M} s_1^2 + \frac{1}{2} \frac{m_2 (M - m_2)}{M} s_2^2 + \frac{1}{2} \frac{m_3 (M - m_3)}{M} s_3^2 + \frac{1}{2} \frac{m_4 (M - m_4)}{M} s_4^2 + A \mathbf{g}_1 \cdot \mathbf{g}_2 + B \mathbf{g}_1 \cdot \mathbf{g}_3 + C \mathbf{g}_2 \cdot \mathbf{g}_3 \]

\[ M = m_0 + m_1 + m_2 + m_3, \quad \text{where } A, B, C \text{ are constants that depend on the masses of the particles.} \]

For the N-body problem we get:

\[ T = \frac{1}{2} \frac{MG^2}{M} + \frac{1}{2} \sum_{i=1}^{N-1} \frac{m_i (M - m_i)}{M} s_i^2 + \text{cross terms}, \quad M = \sum_{i=0}^{N-1} m_i \]

The kinetic energy in the centre of mass frame appears to contain cross terms that represent the dynamic interaction among the reduced particles. These are the scalar product terms. However, interaction problems are formulated in the phase space of the interaction and the molecular velocities of the interaction contribute to the dimensions of this phase space. Therefore, within the phase space the molecular velocities of the interaction are orthogonal to one another. If we transform these velocities to the centre of mass frame it follows that the velocities of the reduced particles will be orthogonal to one another as well as to the centre of mass velocity. Hence the cross terms in the kinetic energy become zero. The kinetic energy simplifies to:

\[ T = \frac{1}{2} \frac{MG^2}{M} + \sum_{i=1}^{N-1} \frac{m_i (M - m_i)}{M} s_i^2 + \text{cross terms}, \quad M = \sum_{i=0}^{N-1} m_i \]  \hspace{1cm} (N - body reduced particles), \hspace{0.5cm} M = \sum_{i=0}^{N-1} m_i \]

where \( e_G \) is the centre of mass energy and \( e_i \) is the translational energy of a reduced particle.

Equation (6) shows that the kinetic energy consists of contributions from the centre of mass as well as from each reduced particle. Note also that the mass that appears in the kinetic energy is that of the N-body reduced particle, not that of the two-body reduced particle used in deflection angle calculations.

To determine the post-collision relative speeds we calculate the energy exchange among the reduced particles and the centre of mass. We include the centre of mass only if an external force acts on the system, as then the centre of mass accelerates through the collision. This calculation will also give rise to a post-collision centre of mass speed, but we ignore this – choosing to calculate the centre of mass motion according to equation (3). We model the energy exchange in Part II.

\[ \text{X. MODEL PARAMETER DETERMINATION} \]

The single parameter in the approximate scattering model can be determined by matching results from three- or four-body scattering experiments. Such an experiment may involve firing three or four beams so that their paths cross at a test point in space. The scattering patterns and cross sections are measured and are used to determine the model parameter.

\[ \text{XI. NUMERICAL SIMULATIONS} \]

Although the deflection angle formulae appear complicated they have the same form as the two-body result. For simple molecular potentials these formulae can be evaluated analytically, as for two-body collisions. For complicated potentials the best policy is to compute the deflection angles once and then to store the results in a look-up table which can be interpolated from during DSMC computations. This way the time penalty for calculating deflection angles during DSMC studies is much reduced. Phillips and Beightler (Ref. 5) have discussed beta distribution sampling.
XII. REFERENCES


Figures

(a) Showing all the forces and separations. The motion reduces to that of two reduced particles $m_0$, formed between particles 0 and 1, and $m_2$, formed between particles 0 and 2. In addition to the primary deflection angle caused by the force between the particles there are secondary deflection angles as well as a deflection of the collision plane caused by the other forces.

(b) Three bodies: the effects of $F_{02}$ on the motion of the reduced particle $m_0$. This force induces a secondary deflection angle as well as a deflection of the collision plane.

(c) Three bodies: the effects of $F_{12}$ on the motion of the reduced particle $m_0$. This force also induces a secondary deflection angle as well as a deflection of the collision plane.
Fixed centre of force for 3D motion of reduced particle. This motion can be resolved in the horizontal plane ABCDEF and in the vertical plane AGHIJB (see dotted trajectories).

Figure 2. Many-body collision reduced to the 3D central force motion of a number of reduced particles. Each reduced particle interacts in 3D with a fixed centre of force which causes deflection of the particle in space. This deflection can be resolved in two planes, one showing a deflection in $c$ and the other showing a deflection of the collision plane in $e$.

Particle of reduced mass approaches the potential field of the rest particle at an impact parameter $b$.

Figure 3. Geometry of many-body scattering in the centre of mass frame.
### TABLE 1. Potential functions and their coefficients for three-body collisions.

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<th>Reduced Particle</th>
<th>Potential</th>
<th>Signed Fraction</th>
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<tr>
<td></td>
<td>( V_{02} )</td>
<td>( m_{b1}/m_0 )</td>
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<td></td>
<td>( V_{12} )</td>
<td>( -m_{b1}/m_1 )</td>
</tr>
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<td>( V_{02} )</td>
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</tr>
<tr>
<td></td>
<td>( V_{01} )</td>
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<td></td>
<td>( V_{12} )</td>
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### TABLE 2. Potential functions and their coefficients for four-body collisions.

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