

COLLISION OF THREE HARD SPHERES

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It is shown that the collision problem with three hard spheres does not have a solution in some circumstances. A solution is obtained only if it is assumed that forces between spheres are continuous.

1. Introduction

A very useful assumption for analysing atom-molecule energy transfer and cross sections is that atoms are hard spheres. A number of relevant informations is obtained from this model, which is primarily due to the fact that in many cases long and medium range forces between atoms do not play significant role in energy transfer. Another reason for its use is that calculations with real potentials are often very lengthy, while this model can give qualitative features of cross section without too much effort. The model has been used for description of various collision processes¹⁻⁵). The use of hard sphere model can also be found in elementary particle physics⁶), although at present time it does not have a more detailed comparison with other dynamical theories in high energy physics. There are some difficulties in this model which we would want to describe. However, before doing this we will review the known facts about the two and three hard sphere scattering problem.

If a sphere of the mass m_1 , and with the initial velocity v_0 , approaches in the head on collision a sphere of the mass m_2 , which is stationary, then after collision the two spheres will have velocities obtained from the set of equations

$$m_1 v_0 = m_1 v_1 + m_2 v_2 \quad (1)$$

$$m_1 \frac{v_0^2}{2} = m_1 \frac{v_1^2}{2} + m_2 \frac{v_2^2}{2}.$$

The first equation is conservation of momentum while the second is conservation of energy. This set solves the collinear two hard spheres problem and the solution is

$$v_1 = \frac{1 - \eta}{1 + \eta} v_0; \quad v_2 = \frac{2}{1 + \eta} v_0 \quad (2)$$

where from now on we will designate by η the ratio $m_2/m_1 = \eta$. As we notice, when $\eta > 1$ i. e. $m_2 > m_1$, the final velocity of the sphere with the mass m_1 is negative, meaning that the sphere is moving in the opposite direction relative to the initial velocity. When $\eta < 1$ its velocity vector is in the same direction as v_0 .

What happens when three spheres are in line and they collide? For simplicity we will assume that two of them have equal mass m_2 , and they are stationary before the collision, while the third one comes from the left and has a mass m_1 and the velocity v_0 . The usual scenario for the solution of this problem is as follows: the sphere m_1 hits one sphere (we will call it sphere 2) and after collision the sphere 2 hits the third sphere (we will call it sphere 3). Therefore, it is assumed that all the three spheres are independent and in a collision only two of them participate, those which are directly involved in the collision.

We can now easily obtain the solution of this problem. After the first collision velocities of the three spheres are

$$v_1^{(1)} = \frac{1 - \eta}{1 + \eta} v_0; \quad v_2^{(1)} = \frac{2}{1 + \eta} v_0; \quad v_3^{(1)} = 0 \quad (3)$$

which were obtained from (2). In the second collision sphere 2 hits sphere 3, and since they have equal mass, by our assumption, the velocities are

$$v_1^{(2)} = \frac{1 - \eta}{1 + \eta} v_0; \quad v_2^{(2)} = 0; \quad v_3^{(2)} = \frac{2}{1 + \eta} v_0. \quad (4)$$

The collision is over if $\eta > 1$, because the sphere 1 is moving to the left, sphere 2 is stationary and the third sphere is moving to the right. Therefore there is no chance that any of the three spheres will collide again.

However, when $\eta < 1$ sphere 1 moves to the right after first collision and hits the second sphere (which is stationary) and after this collision the velocities are

$$v_1^{(3)} = \left(\frac{1 - \eta}{1 + \eta} \right)^2 v_0; \quad v_2^{(3)} = \frac{2(1 - \eta)}{(1 + \eta)^2} v_0; \quad v_3^{(3)} = \frac{2}{1 + \eta} v_0. \quad (5)$$

Since $\eta < 1$ the collision ends here because $v_3^{(3)} > v_2^{(3)} > v_1^{(3)}$. Therefore, the collision of three spheres, in this scenario, has either solution (4) (for $\eta < 1$) or (5) (for $\eta > 1$), and we can say that this problem is solved.

However, in the solution we have neglected a very important case; what happens if the spheres 2 and 3 touch each other before the first collision. In all our previous discussion we have implicitly assumed that the separation between the spheres 2 and 3 is nonzero, but very small. It is obvious that when this gap is zero, the previous solution will not apply because sphere 1 does not hit an object with the mass m_2 i. e. only sphere 2, but an object with the mass $2m_2$. On the other hand, the spheres 2 and 3 are not glued together so that after collision they stay together. In such a case, we cannot apply the model where we can treat the sphere 2 and 3 as one particle.

If we try to solve this problem in the usual way i. e. by considering the laws of conservation, we immediately run into difficulties; there are too few equations for the number of degrees of freedom. On the other hand, if it is to be solved from the dynamic equations i. e. from the equations of motion, we run into difficulty because for the infinitely hard spheres the forces among them have infinite jump below certain intersphere separation.

Similar observation was made by Chapman⁷⁾, who discussed collision of three equal mass spheres in the popular toy: the impact ball apparatus. He found that when two stationary balls of finite elasticity are in contact before collision, the velocities after collision are not given by the Eqs. (4) and (5). This finding was confirmed subsequently in the experiment⁸⁾. However, the limit of the ideally hard spheres was not discussed and also the case of the nonequal masses.

Circumstances where two spheres touch before collision are found in atom molecule collisions because atoms in molecule are bound by intermolecular forces. On this basis one can argue that independent sphere model will not accurately describe this collision, and therefore there is a need to investigate how much the two models differ from each other.

In the following section we will show how to solve this problem if it is assumed that forces between spheres are linear. This is the case when atoms in molecule are initially in the equilibrium position. For small energy transfer they will be «compressed» by such a small amount that harmonic approximation of potential is valid. Harmonic approximation of potential is not valid for large energy transfer, and for this case we will assume that forces between spheres obey general power law.

2. Collision of three soft spheres

Let us assume that the motion of the spheres 1, 2 and 3 is confined to the X -axis and that their respective coordinates are x_1 , x_2 and x_3 . The spheres are aligned from left to right i. e. $x_3 > x_2 > x_1$. The Lagrangian of the system is

$$L = \frac{1}{2} (m_1 \dot{x}_1^2 + m_2 (\dot{x}_2^2 + \dot{x}_3^2)) - V = T - V \quad (6)$$

where the dot designates the time-derivative and V is the potential. It is convenient to work in the relative coordinates so we will define $u_1 = x_2 - x_1$ and $u_2 = x_3 - x_2$, in which case the Lagrangian becomes

$$L = \frac{1}{\Sigma} \left(m_1 m_2 \dot{u}_1^2 + \frac{m_2 (m_1 + m_2)}{2} \dot{u}_2^2 + m_1 m_2 \dot{u}_1 \dot{u}_2 \right) - V \quad (7)$$

where $\Sigma = m_1 + 2m_2$. From (7) we have taken out the term which corresponds to the motion of the center of mass of the whole system.

The equations of motion are in general given by

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}; \quad i = 1, 2, \dots \quad (8)$$

where q_i is a generalized coordinate. In our case $q_1 = u_1$ and $q_2 = u_2$, so that (8) gives

$$\frac{2m_1 m_2}{\Sigma} \ddot{u}_1 + \frac{m_1 m_2}{\Sigma} \ddot{u}_2 = - \frac{\partial V}{\partial u_1} \quad (9)$$

$$\frac{m_2 (m_1 + m_2)}{\Sigma} \ddot{u}_2 + \frac{m_1 m_2}{\Sigma} \ddot{u}_1 = - \frac{\partial V}{\partial u_2}$$

or when we solve the set in the variables u_1 and u_2

$$\ddot{u}_1 = - \frac{1}{\mu} \frac{\partial V}{\partial u_1} + \frac{1}{m_2} \frac{\partial V}{\partial u_2}; \quad \ddot{u}_2 = - \frac{2}{m_2} \frac{\partial V}{\partial u_2} + \frac{1}{m_2} \frac{\partial V}{\partial u_1} \quad (10)$$

where $\mu = m_1 m_2 / (m_1 + m_2)$.

The term V in (7) is the potential energy of the system, which is of the form

$$V = V_{12}(u_1) + V_{23}(u_2) \quad (11)$$

where the indices of potential indicate the spheres. Since the motion of the spheres is confined to only one dimension, the potential V_{13} is strictly zero. This is in accordance with our assumption that the spheres do not interact before they make a physical contact. Therefore, the potentials V_{12} and V_{23} are also strictly zero beyond certain value of separations u_1 and u_2 , which is equal to the sum of the corresponding radii of the spheres. For simplicity we will assume that all spheres have equal radius R , in which case

$$\begin{aligned} V_{12} &= 0; & \text{for } u_1 &> 2R = \sigma \\ V_{23} &= 0; & \text{for } u_2 &> \sigma. \end{aligned} \quad (12)$$

One can show that we obtain identical results if the radii of the spheres are not equal.

When the spheres make a contact i. e. when $u_1 < \sigma$ or $u_2 < \sigma$, we will assume that the potential corresponds to the harmonic oscillator i. e. the force which acts between the neighbouring spheres is linear with the separation u_1 or u_2 . We write

$$V_{12}(u_1) = \frac{C}{2}(\sigma - u_1)^2; \quad \text{for } u_1 < \sigma \quad (13)$$

$$V_{23}(u_2) = \frac{C}{2}(\sigma - u_2)^2; \quad \text{for } u_2 < \sigma$$

where we have assumed that the force constant C is equal for the spheres 1 and 2, and the spheres 2 and 3.

If we define new coordinates $z_1 = \sigma - u_1$ and $z_2 = \sigma - u_2$, the equations of motion are

$$\ddot{x}_1 = -\frac{C}{\mu}z_1 + \frac{C}{m_2}z_2; \quad \ddot{x}_2 = -\frac{2C}{m_2}z_2 + \frac{C}{m_2}z_1 \quad (14)$$

which apply when both $z_1 > 0$ and $z_2 > 0$. The constant C measures the gradient of the force between the spheres. Its value is finite, but we would like to obtain the solution of equations (14) in the limit $C \rightarrow \infty$, which is the limit for the hard spheres. This solution is easily obtained if we first rescale the time and the coordinate variable i. e. if we put

$$t' = t\sqrt{\frac{C}{m_1}}; \quad z'_1 = z_1\sqrt{\frac{C}{m_1}}; \quad z'_2 = z_2\sqrt{\frac{C}{m_1}} \quad (15)$$

in which case (15) becomes

$$\ddot{z}'_1 = -\left(1 + \frac{1}{\eta}\right)z'_1 + \frac{1}{\eta}z'_2; \quad \ddot{z}'_2 = -\frac{2}{\eta}z'_2 + \frac{1}{\eta}z'_1 \quad (16)$$

where the asterisk designates derivative with respect to t' .

The problem which we will consider was stated in the introduction; what is the outcome of collision when the spheres 2 and 3 touch each other before the impact with the sphere 1. The initial conditions at $t = 0$ for this circumstances are: $z'_1 = z'_2 = 0$, $\dot{z}'_1 = v_0$ and $\dot{z}'_2 = 0$. The end of collision is when the coordinates z'_1 and z'_2 become zero again, while the velocities \dot{z}'_1 and \dot{z}'_2 are negative. When this happens we obtain the velocities v_1 , v_2 and v_3 of the spheres 1, 2 and 3, respectively, from the set of equations

$$\begin{aligned} v_2 - v_1 &= -\dot{z}'_1; & v_3 - v_2 &= -\dot{z}'_2 \\ v_0 &= v_1 + \eta(v_2 + v_3). \end{aligned} \quad (17)$$

The last equation is obtained from the motion of the center of mass of the system. The solution of the Eqs. (17) is

$$\begin{aligned} v_1 &= \frac{v_0 + \eta(2z_1^* + z_2^*)}{1 + 2\eta}; & v_2 &= \frac{v_0 - z_1^* + \eta z_2^*}{1 + 2\eta} \\ v_3 &= \frac{v_0 - z_1^* - (1 + \eta)z_2^*}{1 + 2\eta}. \end{aligned} \quad (18)$$

The set of equations (16) can be written in the matrix form

$$\ddot{z}' = -M z' \quad (19)$$

where z' is a column vector with the components z_1' and z_2' , and M is the matrix

$$M = \begin{vmatrix} 1 + \frac{1}{\eta} & -\frac{1}{\eta} \\ -\frac{1}{\eta} & \frac{2}{\eta} \end{vmatrix}. \quad (20)$$

A general solution of (19) is

$$z' = \sin(M^{1/2} t') A + \cos(M^{1/2} t') B \quad (21)$$

where A and B are constant vectors. When we consider the initial conditions, then

$$z' = M^{-1/2} \sin(M^{1/2} t') V_0 \quad (22)$$

where V_0 is the column vector with the elements v_0 and 0. In a more explicit form, the solution is

$$\begin{aligned} z_1' &= \frac{v_0}{1+a} \left(\frac{\sin(\sqrt{\lambda_1} t')}{\sqrt{\lambda_1}} + a \frac{\sin(\sqrt{\lambda_2} t')}{\sqrt{\lambda_2}} \right) \\ z_2' &= \frac{v_0 b}{1+a} \left(\frac{\sin(\sqrt{\lambda_1} t')}{\sqrt{\lambda_1}} - \frac{\sin(\sqrt{\lambda_2} t')}{\sqrt{\lambda_2}} \right) \end{aligned} \quad (23)$$

where

$$a = \frac{\lambda_1 - 1 - 1/\eta}{1 + 1/\eta - \lambda_2}; \quad b = \eta(1 + 1/\eta - \lambda_1) \quad (24)$$

and

$$\lambda_{1,2} = \frac{1}{2} (1 + 3/\eta) \pm \frac{1}{2} ((1 - 1/\eta)^2 + 4/\eta^2)^{1/2}. \quad (25)$$

In the next step we look for the first positive zero of z'_1 and z'_2 , in the variable t' . Usually we will obtain two different values of t' , meaning that when one coordinate is zero, the collision ended for the relevant spheres, while the other two spheres are still in contact. For example, if we find that for $t' = t_0$ the coordinate z'_1 is zero and $z'_2 > 0$, the spheres 1 and 2 have separated, while the spheres 2 and 3 are still interacting. The set of Eqs. (16) no longer describes this situation and we must switch to a new set of equations appropriate for this case, which is

$$z^{**'}_1 = \frac{1}{\eta} z_2; \quad z^{**'}_2 = -\frac{2}{\eta} z'_2. \tag{26}$$

The solution is

$$z'_1 = \frac{1}{2} (z'^0_2 - z'_2) + (z^{*0}_1 + \frac{1}{2} z^{*0}_2)(t' - t'_0) \tag{27}$$

$$z'_2 = \sqrt{\frac{\eta}{2}} z^{*0}_2 \sin\left(\sqrt{\frac{2}{\eta}}(t' - t'_0)\right) + z'^0_2 \cos\left(\sqrt{\frac{2}{\eta}}(t' - t'_0)\right)$$

where z'^0_1, z^{*0}_1, z'^0_2 and z^{*0}_2 are the values of the appropriate variables at $t' = t'_0$.

We now look for the value of t' for which z'_2 is zero, which indicates that the collision ended completely. z^{*0}_1 and z^{*0}_2 are then calculated and used in (18) to obtain velocities of the spheres after collision.

Similar considerations apply when $z'_2 = 0$ for $t' = t'_0$, except that the role of z'_1 and z'_2 is interchanged.

The question is what happens to solution when we take the limit $C \rightarrow \infty$. The »time« t'_0 is independent of C because it corresponds to the instant when either z'_1 or z'_2 is zero (the condition which is independent of C) and the solution (23) is independent of C . Therefore when $C \rightarrow \infty$ the real time t_0 , which is given by (15), goes to zero, meaning that for hard spheres the time which the spheres spend in contact goes to zero, which is plausible conclusion. Likewise the »coordinates« z'_1 and z'_2 are independent of C and when $C \rightarrow \infty$ the real coordinates z_1 and z_2 go to zero. This only reflects the fact that hard spheres are incompressible. Because of scalling (15) final »velocities« z^{*0}_1 and z^{*0}_2 , which we obtain from (27), equal to real velocities \dot{z}'_1 and \dot{z}'_2 , and therefore they are finite. These velocities are therefore also valid in the limit $C \rightarrow \infty$ and they represent solution of the hard sphere problem.

3. Discussion

We will here calculate final velocities v_1, v_2 and v_3 of the three spheres from the equations of motion, and compare results with the hard sphere model, summarized in Eqs. (4) and (5). Final distribution of velocities depends only on the ratio $\eta = m_2/m_1$, and therefore we will calculate this distribution as a function of this parameter. For the initial velocity we will take $v_0 = 1$, since v_1, v_2 and v_3 are

directly proportional to v_0 . In Fig. 1 we show results of these calculations. By the broken line we indicate results of Eqs. (4) and (5), while the full line shows results of the model with the linear force.

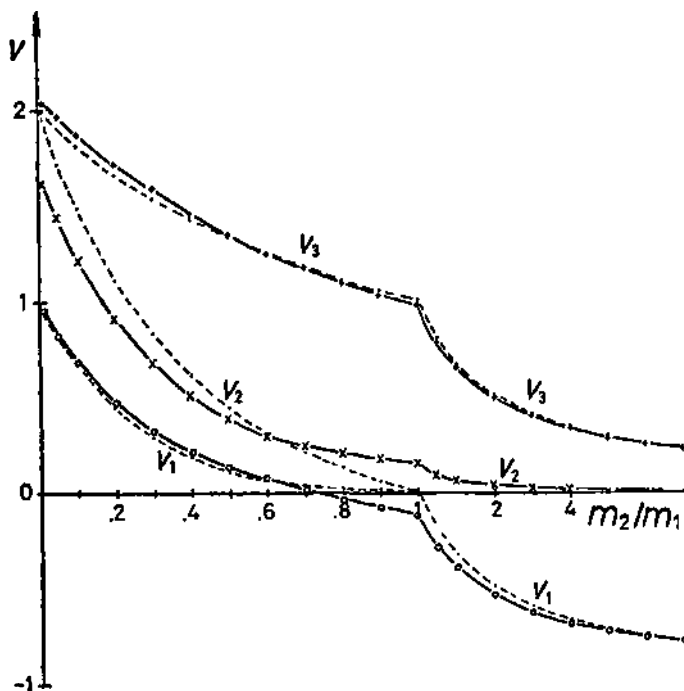


Fig. 1. Final velocities v_1 , v_2 and v_3 of the spheres 1, 2 and 3, respectively, when the sphere 1 has initial velocity $v_0 = 1$ (arb. units) and the spheres 2 and 3 are in contact before collision. The full line represents calculation if the forces among the spheres are linear in the intersphere separation. The broken line represents calculation from Eqs. (4) and (5).

We notice that there is a difference between these two results. The smallest difference is for v_3 , however, both models correctly predict the limit $\eta \rightarrow \infty$ i. e. $m_2 \gg m_1$. The limit $\eta \rightarrow 0$ i. e. $m_2 \ll m_1$ of v_2 and v_3 is different in the two models. A very interesting case is when $\eta = 1$ i. e. $m_2 = m_1$. The hard sphere model predicts that the velocities v_1 and v_2 will be strictly zero while $v_3 = v_0$. However, in reality this is not the case: the velocity v_1 is negative, about 13% of v_0 , while the velocity v_2 is positive, about 15% of v_0 .

The question is can we say anything about the outcome of collision if the forces between spheres are not linear. If we assume that the x -dependence of the force is Cx^α , where α is real positive power, then the set of equations (16) becomes

$$\ddot{x}'_1 = -2x'^{\alpha}_1 + x'^{\alpha}_2; \quad \ddot{x}'_2 = -2x'^{\alpha}_2 + x'^{\alpha}_1 \quad (28)$$

where for simplicity we have assumed that all three spheres are identical. It is interesting to notice that the Eqs. (28) are independent of C , which was achieved

by a suitable scalling of the time and coordinates. Therefore the final velocities (18) are also independent of the constant C . They are entirely dependent on the power α .

For a general power α the set of Eqs. (28) cannot be solved analitically. However, certain information about the outcome of collision can be obtained by considering what happens to the spheres just after the collision began.

In vicinity of $t' = 0$ we can write solutions z'_1 and z'_2 as power series in t' and the leading terms are

$$z'_1 = v_0 t' + a_0 t'^n; \quad z'_2 = b_0 t'^n \tag{29}$$

where we have taken into account the initial conditions $z'_1 = z'_2 = \dot{z}'_2 = 0$ and $\dot{z}'_1 = v_0$ at $t' = 0$. The constants n , a_0 and b_0 must be determined. If in (28) z'_1 and z'_2 are replaced by (29) we obtain

$$\begin{aligned} a_0 n(n-1) t'^{n-2} &= -2v_0^\alpha t'^\alpha \\ b_0 n(n-1) t'^{n-2} &= v_0^\alpha t'^\alpha \end{aligned} \tag{30}$$

where only the leading terms on both sides were retained. From (30) we find the parameters in (29)

$$\begin{aligned} n = 2 + \alpha; \quad a_0 &= -2v_0^\alpha / (\alpha + 2)(\alpha + 1) \\ b_0 &= v_0^\alpha / (\alpha + 2)(\alpha + 1). \end{aligned} \tag{31}$$

The parameters indicate that immediately after collision the time dependence of the coordinates is

$$\begin{aligned} z'_1 &\sim v_0 t' - 2t'^2 (v_0 t')^\alpha / (\alpha + 2)(\alpha + 1) \\ z'_2 &\sim t'^2 (v_0 t')^\alpha / (\alpha + 2)(\alpha + 1). \end{aligned} \tag{32}$$

In this approximation v_3 , which is given by (18), is negligible so that we can say that the sphere 3 does not move immediately after collision started. This is especially the case for large α when the sphere 3 is stationary during the time the spheres 1 and 2 interact. Physically this is understandable because for the set of Eqs. (28) is $\dot{z}'_1 = 0$ and $\dot{z}'_2 = 0$ for $|z'_1|, |z'_2| < 1$. As the time increases the coordinate z'_1 becomes larger than 1 for $t' > 1/v_0$, while z'_2 remains zero. The set of Eqs. (28) now formally describe collision of hard spheres when the spheres 2 and 3 are not initially in contact. In such a case we know the outcome of collision; it is described by the Eqs. (4) and (5). Therefore, the spheres 1, 2 and 3 act as if their radius has shrunk by $\Delta z' = 1/2$.

Indeed when the set of equations (28) was solved numerically for increasing values of α the velocities v_1, v_2 and v_3 approached the values 0, 0 and 1, respectively, as predicted by Eqs. (4). For example, when $\alpha = 2$ the velocities are; $v_1 = -0.0379$, $v_2 = 0.0394$ and $v_3 = 0.9985$, while for $\alpha = 4$ they are; $v_1 = -0.0028$, $v_2 = 0.0028$ and $v_3 = 0.9999$, all in units of v_0 .

In the other extreme for $\alpha \rightarrow 0$ we can find approximate solution from the physical considerations. Let us look at the equation for z'_2 in (28). We will assume that for a small $t' > 0$ both z'_1 and z'_2 are positive (this only reflects the fact that all three particles interact). In such a case the sign of the second derivative z''_2 is very sensitive to the relative magnitudes of z'_1 and z'_2 . This is because any positive number raised to the power α is almost unity, and therefore as t increases from zero a very small excessive increase of z'_1 makes the derivative z''_2 large and positive. Since z'_2 and z''_2 are small for $t \approx 0$ the sign of z''_2 means that z'_2 increases. As z'_2 acquires large value (compared to z'_1) the second derivative becomes negative and z'_2 eventually decreases. Since α is small the change of sign of z''_2 is almost discontinuous around the values of z'_1 and z'_2 for which $z'^{\alpha}_1 = 2z'^{\alpha}_2$, and therefore the solution z'_2 stabilizes around the value for which $z''_2 \approx 0$ i. e. $z'_2 \approx 2^{-1/\alpha}$, $z'_1 \approx 0$. The equation for z'_1 is then $z'_1 \approx -\frac{3}{2}z'^{\alpha}_1 \approx -\frac{3}{2}$ with the solution

$$z'_1 \approx -\frac{3}{4}t'^2 + v_0 t'. \quad (33)$$

For $t' = \frac{4}{3}v_0$ all three spheres separate since $z'_1 = 0$ and $z'_2 \approx z'_1 = 0$ and therefore collision ends. At that moment $z'_1 \approx -2v_0$ and $z'_2 \approx 0$, from which it follows that $v_1 = -\frac{1}{3}v_0$, $v_2 = \frac{2}{3}v_0$ and $v_3 = \frac{2}{3}v_0$. But this means that when $\alpha \approx 0$ the spheres 2 and 3 act in collision with the sphere 1 as one particle. Both spheres stay together even after collision. That our qualitative conclusions are correct we have tested by numerical integration of the equations (28) for small α . For $\alpha = 0.5$ we obtained: $v_0 = -0.2383$, $v_2 = 0.3219$ and $v_3 = 0.9163$, while for $\alpha = 0.25$ these velocities are: $v_1 = -0.3218$, $v_2 = 0.5534$ and $v_3 = 0.7684$, all in units of v_0 . For even smaller α i. e. $\alpha = 0.1$, these results are identical to our prediction to at least 4 significant figures.

Our discussion was primarily motivated by the question what is the outcome of collision if the power law of the interaction between the spheres is changed. We have found that the final velocities of spheres do not depend on the coupling constant C in the power law Cz , but on the value of α . This conclusion also applies in the limit $C \rightarrow \infty$, which means hard spheres. It follows from this that in atom-molecule collisions the final velocity distribution of atoms depends on the form of interaction between individual atoms. For light incoming atoms this dependence is small, but for atoms of comparable mass the final velocities will depend critically on α . For low energy scattering we can assume that $\alpha \approx 1$, but for higher energy scattering α is larger.

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SUDAR TRI ČVRSTE LOPTE

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Može se pokazati da sudar tri čvrste lopte u nekim slučajevima nema rješenja. Rješenje se dobije jedino u slučaju ako se pretpostavi da su sile među loptama kontinuirane.