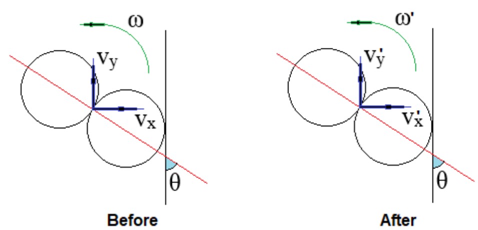
Physics Courseware
Classical Mechanics

Scattering of a diatomic molecule

Problem 1.- Consider a diatomic molecule to be approximated by two solidly joined spheres moving in two dimensions. Knowing its initial velocity (v_x,v_y) and ω, calculate the final velocities after elastically hitting a smooth wall at angle θ as shown below. We take the case when the vibrational state remains the same, so the molecule can be treated as a solid object.



Solution: If the wall is smooth, it cannot apply a vertical force on the molecule, so the vertical velocity will remain the same.

$$v'_y = v_y \tag{1}$$

Because the collision is elastic, kinetic energy is conserved, which means that

$$\frac{1}{2}Mv_x^{\,2} + \frac{1}{2}I\omega^2 = \frac{1}{2}Mv'^{\,2}_x + \frac{1}{2}I\omega'^2 \tag{2}$$

Next, we consider the effect of the impulse (force integrated over time) that the wall applies on the molecule.

$$Ft = M(v'_x - v_x) \tag{3}$$

$$Ftr\cos\theta = I(\omega' - \omega) \tag{4}$$

We can eliminate Ft in the equations (3) and (4) above, obtaining

$$Mr\cos\theta(v'_x - v_x) = I(\omega' - \omega) \tag{5}$$

The energy equation (2) can be rewritten as

$$M(v_x - v'_x)(v_x + v'_x) = I(\omega' - \omega)(\omega' + \omega) \tag{6}$$

And dividing by the previous equation we get

$$\frac{M(v_x - v'_x)(v_x + v'_x)}{Mr\cos\theta(v'_x - v_x)} = \frac{I(\omega' - \omega)(\omega' + \omega)}{I(\omega' - \omega)} \tag{7}$$

implying that

$$v_x + v'_x = -r\cos\theta(\omega' + \omega) \tag{8}$$

Replacing this last equation (8) in (5) to solve for the angular velocity:

$$\omega' = \frac{I - Mr^2\cos^2\theta}{I + Mr^2\cos^2\theta}\omega - \frac{2Mr\cos\theta}{I + Mr^2\cos^2\theta}v_x \tag{9}$$

And the horizontal velocity

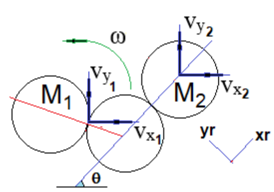
$$v'_x = \frac{Mr^2\cos^2\theta - I}{Mr^2\cos^2\theta + I}v_x - \frac{2Ir\cos\theta}{Mr^2\cos^2\theta + I}\omega \tag{10}$$

As an example, taking $I = 2mr^2$ and $M = 2m$, we get

$$v'_x = \frac{\cos^2\theta - 1}{\cos^2\theta + 1}v_x - \frac{2r\cos\theta}{1+\cos^2\theta}\omega \tag{11}$$

$$\omega' = \frac{1-\cos^2\theta}{1+\cos^2\theta}\omega - \frac{2\cos\theta}{1+\cos^2\theta}\frac{v_x}{r} \tag{12}$$

Problem 2.- Next we treat the problem of a collision between a diatomic molecule and an atom (in two dimensions). The molecule again is approximated by two solidly joined smooth spheres of mass M_1 each and the atom by a smooth sphere of mass M_2. Knowing its initial velocities (v_{x1},v_{y1}), ω and (v_{x2},v_{y2}), calculate the final velocities after the elastic collision as shown below. Once again, assume no energy is transferred to vibrational degrees of freedom, so the molecule behaves as a rigid body.



Solution: Since spheres are smooth, there can only be force along the direction of the centers of the two spheres in contact, so the component of the velocities orthogonal to that direction will remain the same. To take advantage of this, we can re-write the velocities in the rotated set of axes (xr, yr) shown above, then:

$$v'_{yr1} = v_{yr1} \tag{1}$$

$$v'_{yr2} = v_{yr2} \tag{2}$$

Because the collision is elastic, kinetic energy is conserved, which means that

$$\frac{2}{2}M_1 v_{xr1}^{\ 2} + \frac{1}{2}I\omega^2 + \frac{1}{2}M_2 v_{xr2}^{\ 2} = \frac{2}{2}M_1 v'_{xr1}{}^2 + \frac{1}{2}I\omega'^2 + \frac{1}{2}M_2 v'_{xr2}{}^2 \qquad (3)$$

Simplifying

$$2M_1 v_{xr1}^{\ 2} + I\omega^2 + M_2 v_{xr2}^{\ 2} = 2M_1 v'_{xr1}{}^2 + I\omega'^2 + M_2 v'_{xr2}{}^2 \qquad (4)$$

Linear momentum has to be conserved, which indicates that

$$2M_1 v_{xr1} + M_2 v_{xr2} = 2M_1 v'_{xr1} + M_2 v'_{xr2} \qquad (5)$$

The condition for total angular momentum conservation means that

$$2M_1 v_{xr1} b + I\omega = 2M_1 v'_{xr1}\, b + I\omega' \qquad (6)$$

Where we introduce the variable b, which is the distance from the center of mass of the diatomic molecule to the line that passes through the centers of the spheres in contact. Its sign is chosen to indicate a counterclockwise (positive) or clockwise (negative) angular momentum.

We have equations that relate the impulse of the force with the change in linear and angular momentum for the diatomic molecule

$$Ft = 2M_1(v'_{xr1} - v_{xr1}) \qquad (7)$$
$$Ftb = I(\omega' - \omega) \qquad (8)$$

After eliminating Ft we get

$$I(\omega' - \omega) = -2M_1 b(v'_{xr1} - v_{xr1}) \qquad (9)$$

We can use these equations to eliminate ω' in the kinetic energy equation by substituting

$$\omega' = \omega - \frac{2M_1 b}{I}(v'_{xr1} - v_{xr1}) \qquad (10)$$

Obtaining

$$2M_1 v_{xr1}^{\ 2} + I\omega^2 + M_2 v_{xr2}^{\ 2} = 2M_1 v'_{xr1}{}^2 + I\left(\omega - \frac{2M_1 b}{I}(v'_{xr1} - v_{xr1})\right)^2 + M_2 v'_{xr2}{}^2 \qquad (11)$$

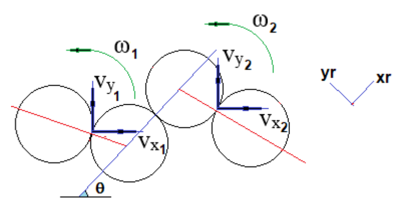
One solution of this quadratic equation is the trivial one, where the velocities are the same as before the collision. The other solution is:

$$v'_{xr1} = \frac{2M_1\left(M_2b^2+I\right)-M_2I}{2M_1\left(M_2b^2+I\right)+M_2I}v_{xr1} + \frac{2M_2I\left(v_{xr2}+b\omega\right)}{2M_1\left(M_2b^2+I\right)+M_2I} \quad (12)$$

$$v'_{xr2} = \frac{M_2(2M_1b^2+I)-2M_1I}{M_2(2M_1b^2+I)+2M_1I}v_{xr2} + \frac{4M_1I(v_{xr1}-b\omega)}{2M_1\left(M_2b^2+I\right)+M_2I} \quad (13)$$

$$\omega' = \frac{\left(2M_1+M_2\right)I-2M_1M_2b^2}{\left(2M_1+M_2\right)I+2M_1M_2b^2}\omega - \frac{4M_2M_1b(v_{xr2}-v_{xr1})}{\left(2M_1+M_2\right)I+2M_1M_2b^2} \quad (14)$$

Problem 3.- Consider now a collision between two diatomic molecules (in two dimensions) again approximated by solidly joined smooth spheres. Knowing its initial velocities (v_{x1},v_{y1}), ω_1, (v_{x2},v_{y2}) and ω_2, calculate the final velocities after the elastic collision as shown below. Once again, assume no energy is transferred to vibrational degrees of freedom, so the molecules behave as rigid bodies.



Solution: If the spheres are smooth, there can only be force along the direction of the centers of the two spheres in contact, so the component of the velocities orthogonal to that direction will remain the same. To take advantage of this, we can re-write the velocities in the rotated set of axes (xr, yr) shown above, then:

$$v'_{yr1} = v_{yr1} \quad (1)$$

$$v'_{yr2} = v_{yr2} \quad (2)$$

Because the collision is elastic, kinetic energy is conserved, which means that

$$\frac{1}{2}Mv_{xr1}^{\ 2} + \frac{1}{2}I\omega_1^2 + \frac{1}{2}Mv_{xr2}^{\ 2} + \frac{1}{2}I\omega_2^2 = \frac{1}{2}Mv'_{xr1}{}^2 + \frac{1}{2}I\omega'_1{}^2 + \frac{1}{2}Mv'_{xr2}{}^2 + \frac{1}{2}I\omega'_2{}^2 \quad (3)$$

Simplifying

$$Mv_{xr1}^{\ 2} + I\omega_1^2 + Mv_{xr2}^{\ 2} + I\omega_2^2 = Mv'_{xr1}{}^2 + I\omega'_1{}^2 + Mv'_{xr2}{}^2 + I\omega'_2{}^2 \quad (4)$$

Linear momentum has to be conserved, which indicates that

$$v_{xr1} + v_{xr2} = v'_{xr1} + v'_{xr2} \quad (5)$$

The condition for total angular momentum conservation means that

$$Mv_{xr1}b_1 + I\omega_1 + Mv_{xr2}b_2 + I\omega_2 = Mv'_{xr1}\,b_1 + I\omega'_1 + Mv'_{xr2}\,b_2 + I\omega'_2 \qquad (6)$$

Where we introduce the variables b_1 and b_2, which are the distances from the center of mass of each molecule to the line that passes through the centers of the spheres in contact. Their signs are chosen to indicate a counterclockwise (positive) or clockwise (negative) angular momentum.

We have equations that relate the impulse of the force with the change in linear and angular momentum. For example for molecule 1

$$Ft = M(v'_{xr1} - v_{xr1}) \qquad (7)$$

$$Ftb_1 = I(\omega'_1 - \omega_1) \qquad (8)$$

After eliminating Ft we get for the two molecules

$$I(\omega'_1 - \omega_1) = Mb_1(v'_{xr1} - v_{xr1}) \qquad (9)$$

$$I(\omega'_2 - \omega_2) = Mb_2(v'_{xr2} - v_{xr2}) \qquad (10)$$

We can use these equations to eliminate ω' in the kinetic energy equation by substituting

$$\omega'_1 = \omega_1 + \frac{Mb_1}{I}(v'_{xr1} - v_{xr1}) \qquad (11)$$

$$\omega'_2 = \omega_2 + \frac{Mb_2}{I}(v'_{xr2} - v_{xr2}) \qquad (12)$$

Obtaining

$$\begin{aligned} Mv_{xr1}^2 + I\omega_1^2 + Mv_{xr2}^2 + I\omega_2^2 &= Mv'^2_{xr1} + I\left(\omega_1 + \frac{Mb_1}{I}(v'_{xr1} - v_{xr1})\right)^2 \\ &+ Mv'^2_{xr2} + I\left(\omega_2 + \frac{Mb_2}{I}(v'_{xr2} - v_{xr2})\right)^2 \end{aligned} \qquad (13)$$

One solution of this quadratic equation is the trivial one, where the velocities are the same as before the collision. The other solution is:

$$v'_{xr1} = \frac{M(b_1^2 + b_2^2)v_{xr1} + 2I(v_{xr2} + \omega_2 b_2 - \omega_1 b_1)}{2I + M(b_1^2 + b_2^2)} \qquad (14)$$

$$v'_{xr2} = \frac{M(b_1^2 + b_2^2)v_{xr2} + 2I(v_{xr1} - \omega_2 b_2 + \omega_1 b_1)}{2I + M(b_1^2 + b_2^2)} \qquad (15)$$

$$\omega'_1 = \omega_1 + Mb_1 \frac{2(v_{xr2} - v_{xr1} + \omega_2 b_2 - \omega_1 b_1)}{2I + M(b_1^2 + b_2^2)} \quad (16)$$

$$\omega'_2 = \omega_2 + Mb_2 \frac{2(v_{xr1} - \omega_2 b_2 + \omega_1 b_1 - v_{xr2})}{2I + M(b_1^2 + b_2^2)} \quad (17)$$

As an example, imagine that $I = 2mr^2$ and $M = 2m$, then

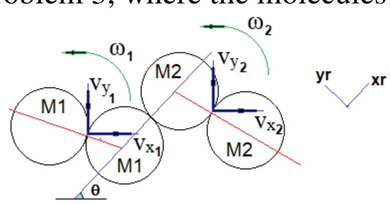
$$v'_{xr1} = \frac{(b_1^2 + b_2^2)v_{xr1} + 2r^2(v_{xr2} + \omega_2 b_2 - \omega_1 b_1)}{2r^2 + b_1^2 + b_2^2} \quad (18)$$

$$v'_{xr2} = \frac{(b_1^2 + b_2^2)v_{xr2} + 2r^2(v_{xr1} - \omega_2 b_2 + \omega_1 b_1)}{2r^2 + b_1^2 + b_2^2} \quad (19)$$

$$\omega'_1 = \omega_1 + 2b_1 \frac{v_{xr2} - v_{xr1} + \omega_2 b_2 - \omega_1 b_1}{2r^2 + b_1^2 + b_2^2} \quad (20)$$

$$\omega'_2 = \omega_2 + 2b_2 \frac{v_{xr1} - \omega_2 b_2 + \omega_1 b_1 - v_{xr2}}{2r^2 + b_1^2 + b_2^2} \quad (21)$$

Problem 4.- A variation of the problem 3, where the molecules are not made of the same atoms.



Solution: We again separate the velocities in components in the rotated set of axes (xr, yr) shown above, then:

$$v'_{yr1} = v_{yr1} \quad (1)$$
$$v'_{yr2} = v_{yr2} \quad (2)$$

Conservation of kinetic energy means that

$$\frac{1}{2}2M_1 v_{xr1}^2 + \frac{1}{2}I_1\omega_1^2 + \frac{1}{2}2M_2 v_{xr2}^2 + \frac{1}{2}I_2\omega_2^2 = \frac{1}{2}2M_2 v'_{xr1}{}^2 + \frac{1}{2}I_2\omega'_1{}^2 + \frac{1}{2}2M_2 v'_{xr2}{}^2 + \frac{1}{2}I_2\omega'_2{}^2 \quad (3)$$

Simplifying

$$2M_1 v_{xr1}^{\ 2} + I_1\omega_1^2 + 2M_2 v_{xr2}^{\ 2} + I_2\omega_2^2 = 2M_1 v'_{xr1}{}^2 + I_2\omega'_1{}^2 + 2M_2 v'_{xr2}{}^2 + I_2\omega'_2{}^2 \qquad (4)$$

Linear momentum has to be conserved, which indicates that

$$M_1 v_{xr1} + M_2 v_{xr2} = M_1 v'_{xr1} + M_2 v'_{xr2} \qquad (5)$$

The condition for total angular momentum conservation means that

$$2M_1 v_{xr1} b_1 + I_1\omega_1 + 2M_2 v_{xr2} b_2 + I_2\omega_2 = 2M_1 v'_{xr1} b_1 + I_1\omega'_1 + 2M_2 v'_{xr2} b_2 + I_2\omega'_2 \qquad (6)$$

b_1 and b_2 are the distances from the center of mass of each molecule to the line that passes through the centers of the spheres in contact. Their signs are chosen to indicate a counterclockwise (positive) or clockwise (negative) angular momentum.

We have equations that relate the impulse of the force with the change in linear and angular momentum. For example for molecule 1

$$Ft = 2M_1(v'_{xr1} - v_{xr1}) \qquad (7)$$

$$Ftb_1 = I_1(\omega'_1 - \omega_1) \qquad (8)$$

After eliminating Ft we get for the two molecules

$$I_1(\omega'_1 - \omega_1) = 2M_1 b_1 (v'_{xr1} - v_{xr1}) \qquad (9)$$

$$I_2(\omega'_2 - \omega_2) = 2M_2 b_2 (v'_{xr2} - v_{xr2}) \qquad (10)$$

We can use these equations to eliminate ω' in the kinetic energy equation by substituting

$$\omega'_1 = \omega_1 + \frac{2M_1 b_1}{I_1}(v'_{xr1} - v_{xr1}) \qquad (11)$$

$$\omega'_2 = \omega_2 + \frac{2M_2 b_2}{I_2}(v'_{xr2} - v_{xr2}) \qquad (12)$$

Obtaining

$$2M_1 v_{xr1}^{\ 2} + I_1\omega_1^2 + 2M_2 v_{xr2}^{\ 2} + I_2\omega_2^2 = 2M_1 v'_{xr1}{}^2 + I_1\left(\omega_1 + \frac{2M_1 b_1}{I_1}(v'_{xr1} - v_{xr1})\right)^2$$
$$+2M_2 v'_{xr2}{}^2 + I_2\left(\omega_2 + \frac{2M_2 b_2}{I_2}(v'_{xr2} - v_{xr2})\right)^2 \qquad (13)$$

One solution of this quadratic equation is the trivial one, where the velocities are the same as before the collision. The other solution is:

$$v'_{xr1} = \frac{\frac{b_1^{\,2}}{I_1} + \frac{b_2^{\,2}}{I_2} + \frac{M_1 - M_2}{2M_2 M_1}}{\frac{b_1^{\,2}}{I_1} + \frac{b_2^{\,2}}{I_2} + \frac{M_1 + M_2}{2M_2 M_1}} v_{xr1} + \frac{1}{M_1} \frac{v_{xr2} + \omega_2 b_2 - \omega_1 b_1}{\frac{b_1^{\,2}}{I_1} + \frac{b_2^{\,2}}{I_2} + \frac{M_1 + M_2}{2M_1 M_2}}$$

$$v'_{xr2} = \frac{\frac{b_1^{\,2}}{I_1} + \frac{b_2^{\,2}}{I_2} + \frac{M_2 - M_1}{2M_1 M_2}}{\frac{b_1^{\,2}}{I_1} + \frac{b_2^{\,2}}{I_2} + \frac{M_2 + M_1}{2M_1 M_2}} v_{xr2} + \frac{1}{M_2} \frac{v_{xr1} + \omega_1 b_1 - \omega_2 b_2}{\frac{b_1^{\,2}}{I_1} + \frac{b_2^{\,2}}{I_2} + \frac{M_2 + M_1}{2M_1 M_2}}$$

$$\omega'_1 = \omega_1 + \frac{2b_1}{I_1} \frac{v_{xr2} - v_{xr1} + \omega_2 b_2 - \omega_1 b_1}{\frac{b_1^{\,2}}{I_1} + \frac{b_2^{\,2}}{I_2} + \frac{M_1 + M_2}{2M_1 M_2}}$$

$$\omega'_2 = \omega_2 + \frac{2b_2}{I_2} \frac{v_{xr1} - v_{xr2} + \omega_1 b_1 - \omega_2 b_2}{\frac{b_1^{\,2}}{I_1} + \frac{b_2^{\,2}}{I_2} + \frac{M_2 + M_1}{2M_2 M_1}}$$