$$A + BC \rightarrow AB + C$$
Collinear Collision

$$Q_1 = x_c - x_b = R_{bc}$$

$$Q_2 = \tfrac{1}{2}(x_b + x_c) - x_a$$

$$Q_3 = \tfrac{1}{3}(x_a + x_b + x_c)$$

This transformation is not necessary, but does make it slightly easier for follow reactive trajectories

$$x_c = \tfrac{1}{2}Q_1 + \tfrac{1}{3}Q_2 + Q_3$$

$$x_b = -\tfrac{1}{2}Q_1 + \tfrac{1}{3}Q_2 + Q_3$$

$$x_a = -\tfrac{2}{3}Q_2 + Q_3$$

$$H = \frac{Pa^2}{2m} + \frac{Pb^2}{2m} + \frac{Pc^2}{2m} + V(x_a, x_b, x_c) \rightarrow \tfrac{1}{2m}\left(\tfrac{1}{2}P_1^2 + \tfrac{2}{3}P_2^2 + 3P_3^2\right) + V(R_{ab}, R_{bc}, R_{ac})$$

$$\left.\begin{aligned} \frac{\partial P_1}{\partial t} &= -\frac{\partial H}{\partial Q_1} \\ \frac{\partial P_2}{\partial t} &= -\frac{\partial H}{\partial Q_2} \\ \frac{\partial P_3}{\partial t} &= -\frac{\partial H}{\partial Q_3} \end{aligned}\right\} \quad \frac{\partial P_i}{\partial t} = -\frac{\partial H}{\partial Q_i}$$

Hamiltonian approach to defining the quantities needed to solve the differential eaquation.

$$\left.\begin{aligned} \frac{\partial Q_2}{\partial t} &= \frac{1}{2m}P_1 \\ \frac{\partial Q_2}{\partial t} &= \frac{1}{2m}\left(\frac{4}{3}P_2\right) \\ \frac{\partial Q_3}{\partial t} &= \frac{1}{2m}(6P_3) \end{aligned}\right\} \quad \frac{\partial Q_i}{\partial t} = \frac{\partial H}{\partial P_i}$$

$$V(R_{ab}, R_{bc}, R_{ac}) = V(x_1, x_2, x_3) = v(Q_1, Q_2, Q_3)$$

Suppose we have a system of Lennard-Jones atoms.

$$V = 4\epsilon\left(\frac{1}{R_{ab}^{12}} - \frac{1}{R_{ab}^{6}}\right) + 4\epsilon\left(\frac{1}{R_{bc}^{12}} - \frac{1}{R_{bc}^{6}}\right) + 4\epsilon\left(\frac{1}{R_{ac}^{12}} - \frac{1}{R_{ac}^{6}}\right)$$

$$\frac{\partial V}{\partial Q_1} = \frac{\partial V_{ab}}{\partial R_{ab}}\frac{\partial R_{ab}}{\partial Q_1} + \frac{\partial V_{bc}}{\partial R_{bc}}\frac{\partial R_{bc}}{\partial Q_i} + \frac{\partial V_{ac}}{\partial R_{ac}}\frac{\partial R_{ac}}{\partial Q_1}, \quad etc.$$