A Three Degree-of-Freedom Index One Saddle–A Saddle-Center-Center Equilibrium Point

We consider a quadratic 3 DoF Hamiltonian:

$$H = \underbrace{\frac{\lambda}{2}\left(p_1^2 - q_1^2\right)}_{H_1} + \underbrace{\frac{\omega_2}{2}\left(p_2^2 - q_2^2\right)}_{H_2} + \underbrace{\frac{\omega_3}{2}\left(p_3^2 - q_3^2\right)}_{H_3}, \quad \lambda,\, \omega_2,\, \omega_3 > 0 \tag{1}$$

with the corresponding Hamilton's equations given by:

$$\begin{aligned}
\dot{q}_1 &= \frac{\partial H}{\partial p_1} = \lambda p_1, \\
\dot{p}_1 &= -\frac{\partial H}{\partial q_1} = \lambda q_1, \\
\dot{q}_2 &= \frac{\partial H}{\partial p_2} = \omega_2 p_2, \\
\dot{p}_2 &= -\frac{\partial H}{\partial q_2} = -\omega_2 q_2, \\
\dot{q}_3 &= \frac{\partial H}{\partial p_3} = \omega_3 p_3, \\
\dot{p}_3 &= -\frac{\partial H}{\partial q_3} = -\omega_3 q_3,
\end{aligned} \tag{2}$$

These equations have an equilibrium point of saddle-center-center equilibrium type (index one saddle) at the origin. Since the Hamiltonians H_1, H_2 and H_3 are uncoupled we can analyze the phase portraits for each separately. As in the previous examples, H_1 corresponds to the ''reactive mode" (trajectories can become unbounded) and H_2 and H_3 are ''bath modes" (trajectories are bounded).

In this system reaction occurs when the q_1 coordinate of a trajectory changes sign. Hence, as in the 2 DoF example, a ''natural" dividing surface would be $q_1 = 0$. This is a five dimensional surface in the six dimensional phase space. We want to examine its' structure more closely and, in particular, its intersection with a fixed 5 dimensional energy surface.

First, note that for reaction to occur we must have $H_1 > 0$. Also, it is clear from the form of H_2 that $H_2 \geq 0$. Therefore, for reaction we must have $H = H_1 + H_2 > 0$. The energy surface is given by:

$$\frac{\lambda}{2}\left(p_1^2 - q_1^2\right) + \frac{\omega_2}{2}\left(p_2^2 + q_2^2,\right) + \frac{\omega_3}{2}\left(p_3^2 + q_3^2,\right) = H_1 + H_2 + H_3 = H > 0, \quad H_1 > 0,\, H_2 \geq 0. \tag{3}$$

The intersection of $q_1 = 0$ with this energy surface is given by:

$$\frac{\lambda}{2}\, p_1^2 + \frac{\omega_2}{2}\left(p_2^2 + q_2^2,\right) + \frac{\omega_3}{2}\left(p_3^2 + q_3^2,\right) = H_1 + H_2 + H_3 = H > 0, \quad H_1 > 0,\, H_2,\, H_3 \geq 0. \tag{4}$$

This is the isoenergetic DS. It has the form of a 3-sphere in the four dimensional $(q_1, p_1, q_2, p_2, q_3, p_3)$ space. It has two ''halves" corresponding to the forward and backward reactions, respectively:

$$\frac{\lambda}{2}\, p_1^2 + \frac{\omega_2}{2}\left(p_2^2 + q_2^2,\right) + \frac{\omega_3}{2}\left(p_3^2 + q_3^2,\right) = H_1 + H_2 + H_3 = H > 0, \quad p_1 > 0, \quad \text{forward DS}, \tag{5}$$

$$\frac{\lambda}{2}\, p_1^2 + \frac{\omega_2}{2}\left(p_2^2 + q_2^2,\right) + \frac{\omega_3}{2}\left(p_3^2 + q_3^2,\right) = H_1 + H_2 + H_3 = H > 0, \quad p_1 < 0, \quad \text{backward DS}. \tag{6}$$

The forward and backward DS ''meet" at $p_1 = 0$:

$$\frac{\omega_2}{2}\left(p_2^2 + q_2^2,\right) + \frac{\omega_3}{2}\left(p_3^2 + q_3^2,\right) = H_2 + H_3 \geq 0, \text{NHIM}, \tag{7}$$

which is a normally hyperbolic invariant 3 sphere. It is *invariant* because on this set $q_1 = p_1 = 0$ and, from (2), if $q_1 = p_1 = 0$ the $\dot{q}_1 = \dot{p}_1 = 0$. Hence, q_1 and p_1 always remain zero, and therefore trajectories with these initial conditions always remain on (7). In other words, it is invariant. It is normally hyperbolic for the same reasons as for our 2 DoF example. The directions normal to (7), i.e. $q_1 - p_1$, are linearized saddle like dynamics.