

## CANONICAL TRANSFORMATION THEORY

A canonical transformation may express new displacements and momenta as functions of both the original displacements and momenta, but is restricted such that it preserves the Hamiltonian form of the differential equations.

Original variables ("old coordinates")

$$H = H(\mathbf{q}, \mathbf{p})$$

$$d\mathbf{q}/dt = \partial H(\mathbf{q}, \mathbf{p})/\partial \mathbf{p} - \mathbf{f}(\mathbf{q}, \mathbf{p}, t)$$

$$d\mathbf{p}/dt = -\partial H(\mathbf{q}, \mathbf{p})/\partial \mathbf{q} + \mathbf{e}(\mathbf{q}, \mathbf{p}, t)$$

The functions  $\mathbf{f}(\mathbf{q}, \mathbf{p}, t)$  and  $\mathbf{e}(\mathbf{q}, \mathbf{p}, t)$  contain the non-conservative and forcing terms and are known as "canonical forces" (an unfortunate historical misnomer).

$$\begin{bmatrix} d\mathbf{q}/dt \\ d\mathbf{p}/dt \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \partial H/\partial \mathbf{q} \\ \partial H/\partial \mathbf{p} \end{bmatrix} + \begin{bmatrix} -\mathbf{f} \\ \mathbf{e} \end{bmatrix}$$

**Symplectic notation:**

$$\mathbf{r} = \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} \quad H = H(\mathbf{r}) \quad \mathbf{G} = \begin{bmatrix} -\mathbf{f} \\ \mathbf{e} \end{bmatrix}$$

$$\mathbf{J} = \begin{bmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{bmatrix}$$

The  $2n \times 2n$  matrix  $\mathbf{J}$  is the so-called *symplectic* matrix. Because  $\mathbf{J} \mathbf{J} = -\mathbf{1}$  it is analogous to the complex number  $j$  (the square root of  $-1$ ). It is also analogous to a  $90^\circ$  rotation matrix.

$$d\mathbf{r}/dt = \mathbf{J} \partial H(\mathbf{r})/\partial \mathbf{r} + \mathbf{G}(\mathbf{r}, t)$$

Change variables ("new coordinates")

$$\mathbf{q} = \mathbf{q}(\mathbf{q}^*, \mathbf{p}^*) \quad \mathbf{p} = \mathbf{p}(\mathbf{p}^*, \mathbf{q}^*)$$

Transform the Hamiltonian by substitution

$$H(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}(\mathbf{q}^*, \mathbf{p}^*), \mathbf{p}(\mathbf{p}^*, \mathbf{q}^*)) = H(\mathbf{q}^*, \mathbf{p}^*)$$

In symplectic notation

$$\mathbf{r} = \mathbf{r}(\mathbf{r}^*)$$

$$H(\mathbf{r}^*) = H(\mathbf{r}^*(\mathbf{r})) = H(\mathbf{r})$$

Differentiate the transformation from  $\mathbf{r}$  to  $\mathbf{r}^*$

$$d\mathbf{r}/dt = \mathbf{T} d\mathbf{r}^*/dt$$

$$\text{where } \mathbf{T} = \partial\mathbf{r}/\partial\mathbf{r}^*$$

is the Jacobian of the "reverse" transformation. Note that  $\mathbf{T}$  is, in general, a function of  $\mathbf{r}^*$ .

By design, the differential equations in the new variables are to have a Hamiltonian form.

$$d\mathbf{r}^*/dt = \mathbf{J} \partial H/\partial\mathbf{r}^* + \mathbf{G}^*$$

Substitute for  $d\mathbf{r}^*/dt$

$$d\mathbf{r}/dt = \mathbf{T} \mathbf{J} \partial H/\partial\mathbf{r}^* + \mathbf{T} \mathbf{G}^*$$

The gradient  $\partial H/\partial\mathbf{r}^*$  may be expressed as follows

$$\partial H/\partial\mathbf{r}^* = \mathbf{T}^t \partial H/\partial\mathbf{r}$$

To justify pre-multiplication by the transpose, expand the partial derivative and note that  $T_{ij} = \partial r_i/\partial r^*_j$

$$\frac{\partial H}{\partial r^*_i} = \sum_j \frac{\partial H}{\partial r_j} \frac{\partial r_j}{\partial r^*_i} = \sum_j \frac{\partial H}{\partial r_j} T_{ji}$$

Therefore

$$d\mathbf{r}/dt = \mathbf{T} \mathbf{J} \mathbf{T}^t \partial H/\partial\mathbf{r} + \mathbf{T} \mathbf{G}^*$$

The Hamiltonian form is to be preserved even if the system is unforced and conservative (i.e.  $\mathbf{G} = 0$ ,  $\mathbf{G}^* = 0$ ) so the *symplectic condition* for a canonical transformation is

$$\mathbf{T} \mathbf{J} \mathbf{T}^t = \mathbf{J}$$

In the general case the relation between the "canonical forces" is

$$\mathbf{G} = \mathbf{T} \mathbf{G}^*$$

We need a transformation from  $\mathbf{G}^*$  to  $\mathbf{G}$ . We could write

$$\mathbf{G}^* = \mathbf{T}^{-1} \mathbf{G}$$

but it is possible to avoid inverting the transformation by rearranging the symplectic condition as follows: Post-multiply by  $\mathbf{T}^t$

$$\mathbf{T} \mathbf{J} = \mathbf{J} \mathbf{T}^t$$

Pre-multiply by  $\mathbf{J}$ , post-multiply by  $-\mathbf{J}$  and use  $\mathbf{J} \mathbf{J} = -\mathbf{1}$

$$\mathbf{J} \mathbf{T} = \mathbf{T}^t \mathbf{J}$$

Pre-multiply by  $\mathbf{T}^t$

$$\mathbf{T}^t \mathbf{J} \mathbf{T} = \mathbf{J}$$

This is an alternative form of the symplectic condition.

Apply it to the transformation of canonical forces by pre-multiplying by  $\mathbf{T}^t \mathbf{J}$  and using  $\mathbf{J}^{-1} = -\mathbf{J}$

$$\mathbf{T}^t \mathbf{J} \mathbf{G} = \mathbf{T}^t \mathbf{J} \mathbf{T} \mathbf{G}^* = \mathbf{J} \mathbf{G}^*$$

$$\mathbf{G}^* = -\mathbf{J} \mathbf{T}^t \mathbf{J} \mathbf{G}$$

The symplectic notation is compact and elegant, but tends to disguise some of the structure of the equations. It can be instructive to express the results in the usual notation. The "reverse" Jacobian  $\mathbf{T}$  is

$$\frac{d}{dt} \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \partial \mathbf{q} / \partial \mathbf{q}^* & \partial \mathbf{q} / \partial \mathbf{p}^* \\ \partial \mathbf{p} / \partial \mathbf{q}^* & \partial \mathbf{p} / \partial \mathbf{p}^* \end{bmatrix} \frac{d}{dt} \begin{bmatrix} \mathbf{q}^* \\ \mathbf{p}^* \end{bmatrix}$$

To express the transformation of canonical forces, note that

$$\mathbf{J} \mathbf{G}^* = \begin{bmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{bmatrix} \begin{bmatrix} -\mathbf{f}^* \\ \mathbf{e}^* \end{bmatrix} = \begin{bmatrix} \mathbf{e}^* \\ \mathbf{f}^* \end{bmatrix}$$

$$\mathbf{J} \mathbf{G} = \begin{bmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{bmatrix} \begin{bmatrix} -\mathbf{f} \\ \mathbf{e} \end{bmatrix} = \begin{bmatrix} \mathbf{e} \\ \mathbf{f} \end{bmatrix}$$

Thus the transformation is

$$\begin{bmatrix} \mathbf{e}^* \\ \mathbf{f}^* \end{bmatrix} = \mathbf{T}^t \begin{bmatrix} \mathbf{e} \\ \mathbf{f} \end{bmatrix} = \begin{bmatrix} [\partial \mathbf{q} / \partial \mathbf{q}^*]^t & [\partial \mathbf{p} / \partial \mathbf{q}^*]^t \\ [\partial \mathbf{q} / \partial \mathbf{p}^*]^t & [\partial \mathbf{p} / \partial \mathbf{p}^*]^t \end{bmatrix} \begin{bmatrix} \mathbf{e} \\ \mathbf{f} \end{bmatrix}$$

Expand

$$\mathbf{e}^* = [\partial \mathbf{q} / \partial \mathbf{q}^*]^t \mathbf{e} + [\partial \mathbf{p} / \partial \mathbf{q}^*]^t \mathbf{f}$$

$$\mathbf{f}^* = [\partial \mathbf{q} / \partial \mathbf{p}^*]^t \mathbf{e} + [\partial \mathbf{p} / \partial \mathbf{p}^*]^t \mathbf{f}$$

Writing the summations explicitly

$$e^*_i = \sum_j (e_j \partial q_j / \partial q^*_i + f_j \partial p_j / \partial q^*_i)$$

$$f^*_i = \sum_j (e_j \partial q_j / \partial p^*_i + f_j \partial p_j / \partial p^*_i)$$