PART III

NUMERICAL AND OTHER TECHNIQUES

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STABILIZATION BY MAKING USE OF A GENERALIZED HAMILTONIAN VARIATIONAL FORMALISM

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ABSTRACT. A generalized Hamiltonian formalism is established which is invariant not only under canonical transformations but under arbitrary transformations. Moreover the dependent variables, coordinates and momenta, as well as the independent variable are allowed to be transformed. This is to say that instead of the physical time t another independent variable s is used, such that t becomes a dependent variable or, more precisely, an additional coordinate. The formalism under consideration permits also to include nonconservative forces.

In case of Keplerian motion we propose to use the eccentric anomaly as the independent variable. By virtue of our generalized point of view a Lyapunov-stable differential system is obtained, such that all coordinates, including the time t, are computed by stable procedures. This stabilization is performed by control terms. As a new result a stabilizing control term also for the time integration is established, such that no longer any kind of time element is needed. This holds true for the usual coordinates as well as for the KS-coordinates.

1. INTRODUCTION

In order to obtain a flexible description of the equations of motion of the two body problem we propose a generalized Hamiltonian variational formalism with the following properties:

1. The formalism is invariant not only under canonical transformations but also under arbitrary transformations of the dependent variables.

2. In order to introduce a new independent variable s (called "fictitious time") instead of the time t the extended phase space is adopted. Hence the physical time t becomes an additional coordinate q_o and therefore its canonical conjugate momentum p_o must be introduced. This momentum is the negative total energy. The aim of all such transformations is to improve the stability behaviour of the differential system as well as to perform an appropriate step-size adaption.

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3. Nonconservative forces are also taken into account and their transformation is performed automatically in the variational formalism.

The generalized formalism proposed in this paper is more general than the classical Hamiltonian theory in analytical dynamics.

2. THE GENERALIZED HAMILTONIAN VARIATIONAL PROBLEM

We introduce the following symbols: q_i generalized coordinates, p_i momenta, $H(p_i,q_i,t)$ Hamiltonian, $P_i(p_k, q_k,t)$ nonconservative forces. The variational principal is then:

$$\int_{t_1}^{t_2} \{\delta[\sum_i p_i \dot{q}_i - H] + \sum_i P_i \delta q_i\}\, dt = 0 \tag{1}$$

$$H = H(p_i,q_i,t)\ , \quad P_i = P_i(p_k,q_k,t), \quad i,k = 1,2,\ldots,n$$

It leads to the following Euler equations:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}\ , \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} + P_i\ , \quad i = 1,2,\ldots,n \tag{2}$$

The variational problem (1) is invariant under arbitrary noncanonical transformations of the dependent variables q_i,p_i. The proof of this statement is not too difficult if Poisson and Lagrange brackets are put in operation.

We illustrate this statement working on the following example: We consider an onedimensional perturbed and damped harmonic oscillator. Equ. (1) is in this case for example:

$$\int_{t_1}^{t_2} \{\delta\left[p\dot{q} - (\frac{p^2}{2m} + \frac{c}{2}\ q^2 + \varepsilon\, \frac{b}{4}\, q^4)\right] - \varepsilon k\ p\ \delta q\}\, dt = 0 \tag{3}$$

with the mass m, ε as the small (dimensionless) perturbing parameter and the constants c,b,k. The equations of motion are:

$$\dot{q} = \frac{p}{m}\ , \quad \dot{p} = -\,cq - \varepsilon\, b\, q^3 - \varepsilon\, k\, p\ . \tag{4}$$

We now perform in (3) the noncanonical transformation introducing amplitude A and angle ψ :

$$q = A \sin\psi\ , \quad p = \sqrt{c\ m}\ \ A \cos\psi. \tag{5}$$

Consequently the variational problem (3) is transformed into

$$\int_{t_1}^{t_2} \{\delta[\sqrt{c}\, m\, A \cos\psi(\dot{A} \sin\psi + \dot{\psi} A \cos\psi)$$
$$- (\frac{c}{2} A^2 + \varepsilon \frac{b}{4} A^4 \sin^4\psi)\,]$$
$$- \varepsilon k \sqrt{c\, m}\, A \cos\psi(\sin\psi \delta A + A \cos\psi\delta\psi)\}dt = 0 \tag{6}$$

The corresponding equations of Euler are

$$\dot{\psi} = \sqrt{\frac{c}{m}} + \frac{\varepsilon\, b}{\sqrt{cm}} A^2 \sin^4\psi + \varepsilon k \cos\psi \sin\psi$$
$$\dot{A} = - \frac{\varepsilon\, b}{\sqrt{c\, m}} A^3 \sin^3\psi \cos\psi - \varepsilon k\, A \cos^2\psi \tag{7}$$

and they are the correct equations of motion of the problem at hand.

3. INTRODUCTION OF A NEW INDEPENDENT VARIABLE

Now we want to introduce a new independent variable s which is linked to the time t by the differential relation

$$\frac{dt}{ds} = t' = \mu > 0, \tag{8}$$

where μ is the scaling function which may depend on all depending variables. In order to incorporate this time transformation into the variaional principle the formalism of the extended phase is appropriate (Stiefel and Scheifele [4]). The physical time t becomes a new coordinate q_o and thus we are forced to introduce its conjugate momentum p_o into the variational principle. The symbol P_o will be explained below. Prime means differentiation with respect to the new independent variable s.

Now our variational principle has the form:

$$\int_{s_1}^{s_2} \{\delta\, [p_o q_o' + \sum_i p_i q_i' - \mu(H + p_o)]$$
$$+ \mu P_o \delta\, q_o + \mu \sum_i P_i \delta\, q_i\}\, ds = 0 \tag{9}$$

$$H = H(p_i, q_i, q_o), \quad P_i = P_i(p_k, q_k, q_o)$$
$$\mu = \mu(p_i, q_i, p_o, q_o) > 0 \qquad i,k = 1,2,\dots,n$$

The variational problem (9) leads to the following set of differential equations:

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$$q_i' = \mu \frac{\partial H}{\partial p_i} + \{H + p_o\} \frac{\partial \mu}{\partial p_i} \tag{10a}$$

$$q_o' = \mu + \{H + p_o\} \frac{\partial \mu}{\partial p_o} \tag{10b}$$

$$p_i' = - \mu \frac{\partial H}{\partial q_i} - \{H + p_o\} \frac{\partial \mu}{\partial q_i} + \mu P_i \tag{10c}$$

$$p_o' = - \mu \frac{\partial H}{\partial q_o} - \{H + p_o\} \frac{\partial \mu}{\partial q_o} + \mu P_o \tag{10d}$$

$$i = 1,2,\ldots,n$$

It is seen that these equations, especially the Equations (10a) and (10c) are only the correct equations of motion provided $\{H + p_o\}$ vanishes on the track. In order to achieve this we do want at first, that $\mu(H + p_o)$ is an integral of motion. This desire is satisfied by putting

$$P_o = - \sum_{j=1}^{n} P_j \frac{\partial H}{\partial p_j} \tag{11}$$

whereby P_o is the (negative) dissipative power. Secondly we choose as initial condition for p_o : $p_o = - H$, at the instant $t = q_o = s = 0$. Then $\mu(H + p_o)$ as well as $\{H + p_o\}$ vanishes on the track. With these prescription it follows at first that p_o is the negative total energy, secondly, Equ. (10b) reduces (in the exact but not in the computed solution) to

$$q_o' = \mu \ ,$$

such that the definition on the time transformation

$$\frac{dt}{ds} = t' = \mu > 0 \tag{8}$$

is included in the differential set (10). Finally Equ. (10d) reads (in the exact but not in the computed solution)

$$p_o' = - \mu \frac{\partial H}{\partial q_o} + \mu P_o$$

which is the wellknown equation of energy.

In practise we do not cancel the terms facterized by $\{H + p_o\}$ in the Equations (10) (called control terms) since they may modify the numerical behaviour during a computer integration in particular they may stabilize.

Remark. In the Lagrangian language of mechanics a compagnion principle

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was published by the author [2]. This principle can be used if the scaling function μ does not depend on the p_i, and the momenta p_i are eliminated directly in the variational problem (9) by the relation

$$q_i' = \mu \frac{\partial H}{\partial p_i} \tag{12}$$

4. EXAMPLE: KEPLERIAN MOTION

Let x_i be rectangular coordinates and p_i the corresponding momenta of a particle of unit mass subjected to the gravitational attraction of a central mass in distrance r. The pertinent Hamiltonian is then:

$$H = \frac{1}{2} \sum_i p_i^2 - \frac{K^2}{r} \quad , \quad r^2 = \sum x_i^2 \; , \quad i = 1,2,3 \tag{13}$$

(K^2: gravitational parameter.)

Let us choose a scaling function

$$\mu = \frac{r}{\sqrt{2p_o}} \tag{14}$$

In this case the fictitious time s is the generalized eccentric anomaly in the sense of Stiefel and Scheifele [4]. It is wellknown that the eccentric anomaly behaves better as independent variable for numerical integration than the time or true anomaly.

Taking into account these assumptions the variational principle (9) becomes for the perturbed motion:

$$\int_{s_1}^{s_2} \{ \delta [p_o x_o' + \sum_i p_i x_i' - (\frac{r}{2\sqrt{2p_o}} \sum_i p_i^2 - \frac{K^2}{\sqrt{2p_o}} + \frac{r}{\sqrt{2p_o}} \varepsilon V + \sqrt{\frac{p_o}{2}} r)] + \frac{r}{\sqrt{2p_o}} \varepsilon P_o \, \delta x_o + \frac{r}{\sqrt{2p_o}} \varepsilon \sum_i P_i \delta x_i \} \, ds = 0 \tag{15}$$

$$p_o = - \sum_j P_j p_j \qquad i,j = 1,2,3$$

Remember that $x_o = q_o = t$ is the physical time, p_o the negative total energy, εP_i are forces, which may not be derivable from a potential, and ε a small (dimensionsless) perturbing parameter.
The Euler equations are:

$$x_i' = \frac{r}{\sqrt{2p_o}} \; p_i \tag{16a}$$

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$$x_o' = \frac{r}{\sqrt{2p_o}} - \left\{\frac{1}{2}\sum_i p_i^2 - \frac{K^2}{r} + \varepsilon V + p_o\right\} \frac{r}{\sqrt{2p_o}^3} =$$

$$= \frac{r}{2\sqrt{2p_o}} - \left[\frac{r}{2}\sum_i p_i^2 - K^2 + \varepsilon r V\right] \frac{1}{\sqrt{2p_o}^3} \tag{16b}$$

$$p_i' = \frac{r}{\sqrt{2p_o}} \left(- \frac{K^2}{r^3} x_i - \varepsilon \frac{\partial V}{\partial x_i}\right) - \left\{\frac{1}{2}\sum_i p_i^2 - \frac{K^2}{r} + \varepsilon V + p_o\right\} \frac{x_i}{r\sqrt{2p_o}} +$$

$$+ \frac{r}{\sqrt{2p_o}} \varepsilon P_i = -\left(\frac{\sum_i p_i^2}{2\sqrt{2p_o}} + \sqrt{\frac{p_o}{2}}\right) \frac{x_i}{r} - \frac{\varepsilon}{\sqrt{2p_o}} \frac{\partial (rV)}{\partial x_i} + \frac{r}{\sqrt{2p_o}} \varepsilon P_i \tag{16c}$$

$$p_o' = \frac{r}{\sqrt{2p_o}} \varepsilon \left[- \frac{\partial V}{\partial x_o} + P_o\right] \tag{16d}$$

The control terms in Equs. (16b) and (16c) are factorized by the same curly brackets. Remember that these control terms (energy relation) vanish provided the integration of the system is exact but that they may modify the behaviour of a numerical integration. In particular we claim that they stabilize the differential system under consideration.

More precisely we prove in the unperturbed case $\varepsilon = 0$ the following statement:

Assumtion. The numerical value of the constant energy p_o is considered as a a priori constant, never varied.

Statement. The system (16a-d) is Lyapunov-stable (for $\varepsilon = 0$)+) with respect to variations of the initial conditions of x_i, x_o, p_i.

Proof: We discuss, at first, the time integration. The system (16) has (in the unperturbed case) the following first integral, where C is an integration constant:

$$x_o = \frac{1}{2p_o}\left[\frac{K^2}{\sqrt{2p_o}} s - \sum_i x_i p_i\right] + C \tag{17a}$$

It is seen by differentiation and inserting appropriately the Equs.(16).

+) Comments: 1. Remember that the classical differential equations of Keplerian motion are unstable. 2. In the perturbed motion p_o is no longer constant thus the strict stability (of the stabilized system (16)) is lost, but the appearing instability is only of the order of magnitude of the perturbing parameter ε (compare the paper of the author [3].

Now we use the basic law of Keplerian motion

$$\sum_i x_i\, p_i = \sqrt{2p_o}\; e \sin E \tag{17b}$$

where E = (s + const) is the eccentric anomaly and e the eccentricity. Equ. (17b) shows that the expression $\sum_i x_i\, p_i$ is pure periodic. From Equ. (17a) it thus follows that variations of the initial conditions of x_i, p_i do influence the time x_o only in pure periodic manner. Therefore x_o is Lyapunov stable.

In order to discuss, secondly, the remaining Equs. (16a), (16c), (16d) we multiply the system (16a-d) by $\sqrt{2p_o}$ and eliminate the momenta p_i. This does not influence the stability behavior. By doing this we obtain:

$$x_i'' - \frac{\sum_j x_j\, x_j'}{r^2}\, x_i' = -\left(\frac{\sum_j x_j'^2}{2r^2} + p_o\right) x_i - r\varepsilon\, \frac{\partial (rV)}{\partial x_i} + r^2 \varepsilon\, P_i \tag{18a}$$

$$p_o' = -\varepsilon \left[r\, \frac{\partial V}{\partial x_o} + \sum_j P_j\, x_j' \right] \tag{18b}$$

$$x_o' = \frac{r}{2} - \left[\frac{\sum_j x_j'^2}{2r} - K^2 + \varepsilon r V \right] \frac{1}{2p_o} \tag{18c}$$

$$i,j = 1,2,3$$

In this system +) the Equs. (18a) and (18b) are identic with the equations for the x_i and p_o ($p_o = h$) discussed in the reference of the author [1] where the Lyapunov-stability of the equations was proved by the Levi-Civita-transformation.

Furthermore the time integration (18c) is stabilized by a control term. This control term is automatically produced by the choose of the scaling function $\mu = \frac{r}{\sqrt{2p_o}}$ instead of $\mu = r$.

We give finally a motivation for our line of approach. In the book Stiefel and Scheifele [4] as well as in the paper of the author [1] the integration of the KS-coordinates as well as usual coordinates x_i with respect to s as the independent variable was stabilized in case of the

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+) Now the independent variable, which we call also s, is no longer the generalized eccentric anomaly, but proportional to this anomaly.

time transformation

$$\frac{dt}{ds} = t' = x_o' = r .$$

But the integration of t(s) was left unstable. In order to remove this instability these publications introduced a time element (or used a t"-equation). The theory above does not need this detour, but stabilizes all integrations including $t = x_o$.

We now list the corresponding stabilized KS-equation. In vector notation we obtain (with $p_o = h$, $x_o = t$):

$$\underline{u}'' + \frac{h}{2}\underline{u} = -\frac{\varepsilon}{4}\frac{\partial}{\partial \underline{u}}(|\underline{u}|^2 V) + \frac{\varepsilon}{2}|\underline{u}|^2 L^T \underline{P} \qquad (19a)$$

$$h' = -\varepsilon|\underline{u}|^2 \frac{\partial V}{\partial t} - 2\varepsilon\,(\underline{u}', L^T \underline{P}) \qquad (19b)$$

$$t' = \frac{1}{2}|\underline{u}|^2 - \left[2\,|\underline{u}'|^2 - K^2 + \varepsilon|\underline{u}|^2 V\right]\frac{1}{2h} \qquad (19c)$$

In case of the canonical KS-theory we have to put

$$\underline{\bar{p}} = 4\,\underline{u}' \qquad (20)$$

and obtain the canonical first order system, which corresponds to the system (16) multiplied by $\sqrt{2p_o} = \sqrt{2h}$.

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