The concept of 'optimal' path in classical mechanics

1986 J. Phys. A: Math. Gen. 19 1333

(http://iopscience.iop.org/0305-4470/19/8/015)

J. Phys. A: Math. Gen. 19 (1986) 1333-1344. Printed in Great Britain

The concept of 'optimal' path in classical mechanics

E J V de Passos†§ and F F de Souza Cruz‡

† Instituto de Física, Universidade de São Paulo, São Paulo, Brasil

‡ Departamento de Física, Universidade Federal de Santa Catarina, Florianópolis, Brasil

Received 22 August 1984, in final form 8 August 1985

Abstract. In this paper we discuss the significance of the concept of 'optimal' path in the framework of classical mechanics. Our derivation of the local harmonic approximation and self-consistent collective coordinate method equations of the optimal path is based on a careful study of the concepts of local maximal decoupling and global maximal decoupling respectively. This exhibits the nature of the differences between these two theories and allows us to establish the conditions under which they become equivalent.

1. Introduction

In a series of papers many authors (Rowe and Bassermann 1976, Rowe 1982, Marumori *et al* 1980, Sakata *et al* 1983, Villars 1977) proposed self-consistent theories of large amplitude collective motion. The starting points of all these developments is the time-dependent Hartree-Fock theory (TDHF) which gives the evolution in time of a Slater determinant. The space of Slater determinants was shown to be a simplectic manifold ('phase space'), M, and the TDHF equations to be identical to Hamilton equations (Rowe *et al* 1980). This makes it possible to cast all these theories in a classical language. Besides, most of the self-consistent theories of large amplitude collective motion simplify the problem further, by the so-called 'adiabatic approximation' (Villars 1977, Goeke and Reinhard 1978). Given a configuration space C of M, its cotangent bundle T^*C is a simplectic manifold. In the adiabatic approximation one assumes that the paths of M of physical interest lie sufficiently close to C that we might neglect, in the Hamitonian, powers of the momentum higher than quadratic. Subject to this restriction and considering the case of only one collective degree of freedom we can state that the basic theoretical problem addressed by these authors is to find an 'optimal' collective path in configuration space. This 'optimal' collective path gives rise to a two-dimensional subspace of the whole phase space and collective motion is identified with the motion of the system constrained to this subspace. The basic difference between these approaches stems from the distinct decoupling properties of its 'optimal' collective path. In the local harmonic approximation (LHA) (Rowe and Bassermann 1976, Rowe 1982), the dynamics is analysed locally, i.e. in the vicinity of a point in the phase space. This analysis establishes, at each point, the decoupling properties of the local degrees of freedom. In other words, one finds the local normal modes. The points where there exists a maximally decoupled local degree of freedom define the LHA optimal path. It is clear that the LHA path is defined on the whole configuration space. However, notice that it was determined by a local analysis of the dynamics. On the other hand, in the self-consistent collective coordinate method (SCC) (Marumori *et al* 1980, Sakata *et al* 1983), one requires a global decoupling. In this

§ Partially supported by CNPq.

case, the dynamics is analysed on the whole phase space, i.e. we consider the Hamilton equations on the whole phase space. The aim of this analysis is to find a maximally decoupled global degree of freedom. This maximally decoupled degree of freedom defines a curve in configuration space which is the 'optimal' path of the SCC method. The subspace of the phase space defined by this 'optimal' path is an invariant two-dimensional surface in phase space (Da Providência and Urbano 1982, Sakata *et al* 1983).

As a consequence of these developments, much progress has been made on the understanding of the concept of 'optimal' path which led to the appearance of applications to nuclear collective motion (Goeke *et al* 1983). In spite of this, many points deserve further clarification. The ones which we believe to be the most important are (i) a better understanding of the concept of local maximal decoupling and (ii) to explain the nature of the difference between the two approaches and to establish the conditions under which they become equivalent. This is done in our paper in the framework of classical mechanics.

In § 2 we present our derivation of the LHA which is based on a careful study of the physical meaning of the concept of local maximal decoupling. In § 3 we present our derivation of the SCC method based on the concept of global maximal decoupling. In § 4 we discuss in what respect these two approaches differ and establish the conditions under which they become equivalent. In § 5 we present our concluding remarks. We think that a detailed investigation of these concepts in the framework of classical mechanics, as is done in our paper, gives useful insights to future applications of these theories to quantum mechanics and many-body problems. One warning before starting: the mathematical level of our paper will be the simplest one compatible with a clear discussion of the concepts involved.

2. Local maximal decoupling and the local harmonic approximation

The configuration space of a classical system of N degrees of freedom is a manifold, C, of dimension N. In the Hamiltonian formalism a dynamical state of the system is a point in the phase space which is the cotangent bundle T^*C of C. If $\boldsymbol{q}=(q^0, q^1, \ldots, q^{N-1})$ are the local coordinates of a point C and $\boldsymbol{p}=(p_0, p_1, \ldots, p_{N-1})$ the components of a covector at this point, the $2N$ numbers $\boldsymbol{q}=(q^0, q^1, \ldots, q^{N-1})$ and $\boldsymbol{p}=(p_0, \ldots, p_{N-1})$ are the canonical coordinates in T^*C. The N numbers $\boldsymbol{p}$ are the momenta associated to the N coordinates $\boldsymbol{q}$.

The canonical transformations which preserve the cotangent bundle structure of C, i.e. keep the Hamiltonian quadratic in the momenta, are the point transformations, defined by

$$\bar{q}^i = f^i(\boldsymbol{q}) \qquad p_i = \sum_{k=0}^{N-1} \frac{\partial f^k}{\partial q^i} \bar{p}_k \tag{2.1a}$$

and its inverse

$$q^i = g^i(\bar{\boldsymbol{q}}) \qquad \bar{p}_i = \sum_{k=0}^{N-1} \frac{\partial g^k}{\partial \bar{q}^i} p_k \tag{2.1b}$$

$$\sum_{k=0}^{N-1} \frac{\partial f^i}{\partial q^k} \frac{\partial g^k}{\partial \bar{q}^j} = \delta^i{}_j.$$

These transformations, equations (2.1), will be the only ones considered in this paper.

The time evolution of the system in the phase space is given by the Hamilton equations

$$\dot{q}^i = \partial H/\partial p_i \qquad \dot{p}^i = -\partial H/\partial q^i \tag{2.2}$$

where

$$H = \tfrac{1}{2}\sum_{i,j} B^{ij}(\boldsymbol{q})p_i p_j + V(\boldsymbol{q}) \tag{2.3}$$

is the Hamiltonian of the system. The transformation (2.1) changes the Hamiltonian (2.3) to

$$\bar{H}(\bar{\boldsymbol{q}}, \bar{\boldsymbol{p}}) = \tfrac{1}{2}\sum_{i,j} \bar{B}^{ij}(\bar{\boldsymbol{q}})\bar{p}_i\bar{p}_j + \bar{V}(\bar{\boldsymbol{q}}) \tag{2.4}$$

where

$$\begin{aligned} &\bar{V}(\bar{\boldsymbol{q}}) = V(\boldsymbol{g}(\bar{\boldsymbol{q}})) \\ &\bar{B}^{ij}(\bar{\boldsymbol{q}}) = \sum_{k,l} \frac{\partial f^i}{\partial q^l}(\boldsymbol{g}(\bar{\boldsymbol{q}}))\frac{\partial f^j}{\partial q^k}(\boldsymbol{g}(\bar{\boldsymbol{q}}))B^{kl}(\boldsymbol{g}(\bar{\boldsymbol{q}})). \end{aligned} \tag{2.5}$$

The equations (2.1) and (2.5) show that, by a change of coordinates, the potential $V(\boldsymbol{q})$ transforms as a scalar, the $B^{ij}(\boldsymbol{q})$ transform as the components of a second-rank tensor and the momenta transform as the components of a covector.

Using the expression (2.3) of the Hamiltonian, the Hamilton equations can be written as

$$\begin{aligned} &\dot{q}^i = \sum_k B^{ik}(\boldsymbol{q})p_k \\ &\ddot{q}^i + \sum_{j,k} \begin{Bmatrix} i \\ jk \end{Bmatrix} \dot{q}^j\dot{q}^k = -\sum_j B^{ij}\frac{\partial V}{\partial q^j}. \end{aligned} \tag{2.6}$$

In equation (2.6) $\{{}^{\,i}_{jk}\}$ are the components of the metric connection (Christoffel symbols) induced by the tensor $B^{ij}(\boldsymbol{q})$ (Synge and Schild 1969):

$$\begin{aligned} &\begin{Bmatrix} i \\ jk \end{Bmatrix} = \sum_l B^{il}(\boldsymbol{q})\frac{1}{2}\left(\frac{\partial M_{lj}(\boldsymbol{q})}{\partial q^k} + \frac{\partial M_{lk}(\boldsymbol{q})}{\partial q^j} - \frac{\partial M_{jk}(\boldsymbol{q})}{\partial q^l}\right) \\ &\sum_l B^{il}(\boldsymbol{q})M_{lk}(\boldsymbol{q}) = \delta^i k. \end{aligned} \tag{2.7}$$

A possible interpretation of what we have just shown is that the trajectory of the system in configuration space is a curve in a Riemannian manifold whose metric tensor is the mass tensor, $M_{ij}(\boldsymbol{q})$.

Our next step is to study the dynamics of the system in the neighbourhood of an equilibrium point, P_0. In this case one has

$$\left(\frac{\partial V}{\partial q^i}\right)_{\boldsymbol{q}=(\boldsymbol{q})_{P_0}} = 0 \qquad (\boldsymbol{p})_{P_0} = \boldsymbol{0} \qquad i = 0, \ldots, N-1$$

where $(\boldsymbol{q})_{P_0}$ and $(\boldsymbol{p})_{P_0}$ are the coordinates and the momenta of the equilibrium point. Near P_0, the Hamiltonian (2.3) can be written as

$$H^L(\boldsymbol{\alpha}, \boldsymbol{\beta}) = (V)_{P_0} + \frac{1}{2}\left(\sum_{i,j} (B^{ij})_{P_0}\beta_i\beta_j + (K_{ij})_{P_0}\alpha^i\alpha^j\right) + \ldots \tag{2.8}$$

where

$$\alpha^i = q^i - (q^i)_{P_0} \qquad \beta_i = p_i,$$

$\boldsymbol{q}$ and $\boldsymbol{p}$ being the coordinates and the momenta of a point in the neighbourhood of P_0. In (2.8) $(V)_{P_0}$, $(B^{ij})_{P_0}$ and $(K_{ij})_{P_0}$ are, respectively, the potential, the contravariant components of the mass tensor and the covariant components of the elastic tensor at P_0,

$$(V)_{P_0} = (V(\boldsymbol{q}))_{\boldsymbol{q}=(\boldsymbol{q})_{P_0}} \tag{2.9a}$$

$$(B^{ij})_{P_0} = (B^{ij}(\boldsymbol{q}))_{\boldsymbol{q}=(\boldsymbol{q})_{P_0}} \tag{2.9b}$$

$$(K_{ij})_{P_0} = \left(\frac{\partial^2 V}{\partial q^i\,\partial q^j}(\boldsymbol{q})\right)_{\boldsymbol{q}=(\boldsymbol{q})_{P_0}} \tag{2.9c}$$

Notice that $(K_{ij})_{P_0}$, given by equation (2.9c), is a tensor only at an equilibrium point. Furthermore, (2.8) defines the local Hamiltonian at the point P_0. Given (2.8) the Hamilton equations near P_0 can be written as

$$\dot{\alpha}^i = \sum_j (B^{ij})_{P_0}\beta_j \qquad \dot{\beta}_i = -\sum_j (K_{ij})_{P_0}\alpha^j. \tag{2.10}$$

It is well known that the Hamiltonian (2.8) can be diagonalised by a linear transformation which defines the normal modes at P_0:

$$\zeta_i = \sum_k a^k_{(i)}\beta_k \qquad \eta^i = \sum_k d^{(i)}_k\alpha^k \tag{2.11a}$$

if

$$\begin{aligned} &\hat{A}\hat{D} = \hat{D}\hat{A} = 1 \\ &\hat{A}^{\mathrm{T}}\hat{K}\hat{A} = \hat{\lambda} \qquad \lambda_{ij} = \lambda_i\delta_{ij} \\ &\hat{A}^{\mathrm{T}}\hat{M}\hat{A} = 1. \end{aligned} \tag{2.11b}$$

In (2.11) $\hat{A}^{\mathrm{T}}$ means the transpose of $\hat{A}$ and $\hat{A}$, $\hat{D}$, $\hat{K}$, $\hat{M}$ are matrices whose elements are $A_{ij} = a^i_{(j)}$, $D_{ij} = d^{(i)}_j$, $K_{ij} = (K_{ij})_{P_0}$ and $M_{ij} = (M_{ij})_{P_0}$.

As $(K_{ij})_{P_0}$ and $(M_{ij})_{P_0}$ are tensors at P_0, the proper frequencies λ_i are independent of the system of coordinates and the $a^k_{(i)}$, $k = 0, \ldots, N-1$ (i fixed) are the contravariant components of a vector at the point P_0, which is the ith local normal mode vector. Using the transformation (2.11), the Hamiltonian and the Hamilton equations near P_0 are given by

$$\bar{H}^L(\boldsymbol{\zeta}, \boldsymbol{\eta}) = (V)_{P_0} + \tfrac{1}{2}\sum_i (\zeta_i^2 + \lambda_i\eta^{i2}) + \ldots \tag{2.12}$$

$$\dot{\eta}^i = \zeta_i \qquad \dot{\zeta}_i = -\lambda_i\eta^i. \tag{2.13}$$

The equations (2.12) and (2.13) show that the local normal modes are decoupled degrees of freedom at P_0. Besides, each pair ζ_i, η^i, $i = 0, \ldots, N-1$ defines, at the point P_0, an invariant plane in phase space. Σ_{P_0} is an invariant plane at the point P_0 if, given that $\boldsymbol{\alpha}_0$, $\boldsymbol{\beta}_0$ is a point in this plane, $\boldsymbol{\alpha}(t)$, $\boldsymbol{\beta}(t)$ remains on it, where $\boldsymbol{\alpha}(t)$, $\boldsymbol{\beta}(t)$ are solutions of the Hamilton equations (2.10) with the initial condition $\boldsymbol{\alpha}_0 = \boldsymbol{\alpha}(t)|_{t=0}$, $\boldsymbol{\beta}_0 = \boldsymbol{\beta}(t)|_{t=0}$. A degree of freedom which at a fixed point is decoupled and defines an invariant plane at this point will be called a maximally decoupled local degree of freedom. Therefore, the normal modes are maximally decoupled degrees of freedom at an equilibrium point.

The question now is to see if one can find maximally decoupled local degrees of freedom, in the sense discussed above, outside an equilibrium point. We will answer this question using an approach identical to the one used previously. In doing so we should take into account the fact that the concepts of local normal modes and proper frequencies must have an intrinsic character. It is clear from our previous discussion that once the coefficients of the quadratic term of the local Hamiltonian are tensors, the above properties are guaranteed to hold. The immediate conclusion from the above observations is that to define the local Hamiltonian at a given point P_0 we should use a system of coordinates for which the covariant derivative is equal to the partial derivative at P_0. A coordinate system with this property always exists and it is called a geodesic coordinate system at the point P_0 (Rowe 1982). However the concept of covariant derivative depends on the metric connection and it is possible to consider several metric connections in the same manifold. Each one will give rise to different definitions of covariant derivative and so different definitions of the local Hamiltonian. Thus, to define the local Hamiltonian outside an equilibrium point one has to choose *a priori* a metric connection. In our case, since the Hamiltonian is quadratic in the momenta, the metric is naturally dictated by the dynamics and it is the metric connection induced by the mass tensor (2.7).

Under the coordinate transformation (2.1), the metric connection transforms according to (Synge and Schild 1969):

$$\overline{\begin{Bmatrix} i \\ jk \end{Bmatrix}} = \sum_{l,m,n} \frac{\partial f^i}{\partial q^l} \frac{\partial g^m}{\partial \bar{q}^j} \frac{\partial g^n}{\partial \bar{q}^k} \begin{Bmatrix} l \\ mn \end{Bmatrix} + \sum \frac{\partial f^i}{\partial q^l} \frac{\partial^2 g^l}{\partial \bar{q}^j \, \partial \bar{q}^k}. \tag{2.14}$$

A geodesic coordinate system at a point P_0 is such that (Synge and Schild 1969):

$$\overline{\begin{Bmatrix} i \\ jk \end{Bmatrix}}_{P_0} = 0. \tag{2.15}$$

The property (2.15) guarantees that the covariant derivative and the partial derivative are equal at the point P_0.

Given that the coordinates $\bar{\boldsymbol{q}}$ are geodesic coordinates at the point P_0 we define the local Hamiltonian as before

$$\bar{H}^L(\bar{\boldsymbol{\alpha}}, \bar{\boldsymbol{\beta}}) = (\bar{V})_{P_0} + \sum_i \left(\frac{\partial \bar{V}}{\partial \bar{q}^i}\right)_{P_0} \bar{\alpha}^i + \frac{1}{2} \sum_{i,j} (\bar{B}^{ij})_{P_0} \bar{\beta}_i \bar{\beta}_j + (\bar{K}_{ij})_{P_0} \bar{\alpha}^i \bar{\alpha}^j + \ldots \tag{2.16}$$

where

$$\bar{\alpha}^i = \bar{q}^i - (\bar{q}^i)_{P_0}$$

$$\bar{\beta}^i = \bar{p}_i - (\bar{p}_i)_{P_0} = \bar{p}_i$$

and

$$\left(\frac{\partial \bar{V}}{\partial \bar{q}^i}\right)_{P_0} = \sum_k \left(\frac{\partial g^k}{\partial \bar{q}^i}\right)_{P_0} \left(\frac{\partial V}{\partial q^k}\right)_{P_0} \tag{2.17a}$$

$$(\bar{B}^{ij})_{P_0} = \sum_{k,l} \left(\frac{\partial f^i}{\partial q^k}\right)_{P_0} \left(\frac{\partial f^j}{\partial q^l}\right)_{P_0} (B^{kl})_{P_0} \tag{2.17b}$$

$$(\bar{K}_{ij})_{P_0} = \left(\frac{\partial^2 \bar{V}}{\partial \bar{q}^i \, \partial \bar{q}^j}\right)_{P_0} = \sum_{k,l} \left(\frac{\partial g^k}{\partial \bar{q}^i}\right)_{P_0} \left(\frac{\partial g^l}{\partial \bar{q}^j}\right)_{P_0} (K_{kl})_{P_0} \tag{2.17c}$$

$$(K_{ij})_{P_0} = \left(\frac{\partial^2 V}{\partial q^i \, \partial q^j}\right)_{P_0} - \sum_m \begin{Bmatrix} m \\ ij \end{Bmatrix}_{P_0} \left(\frac{\partial V}{\partial q^m}\right)_{P_0}. \tag{2.17d}$$

The equations (2.17) deserve several comments. Firstly equation (2.17d) shows that the generalisation of the elastic tensor outside an equilibrium point is the hessian, where the hessian is the second covariant derivative of the potential. Secondly, since P_0 is not an equilibrium point, a linear term appears in the expression of the local Hamiltonian, (2.16). This term depends on the potential gradient field at P_0, as expected. Given (2.16), the Hamilton equations near P_0 can be written as

$$\dot{\bar{\alpha}}^i=\sum_j (\bar{B}^{ij})_{P_0}\bar{\beta}_j \qquad -\dot{\bar{\beta}}_i=\left(\frac{\partial \bar{V}}{\partial \bar{q}^i}\right)_{P_0}+\sum_j (\bar{K}_{ij})_{P_0}\bar{\alpha}^j. \tag{2.18}$$

As before we diagonalise the quadratic term of the Hamiltonian (2.16) by a linear canonical transformation which defines the local normal modes:

$$\eta^i=\sum_k \bar{d}_k^{(i)}\bar{\alpha}^k \qquad \zeta_i=\sum_k \bar{a}_{(i)}^k\bar{\beta}_k$$

if

$$\bar{a}_{(i)}^k=\sum_j \left(\frac{\partial f^k}{\partial q^j}\right)_{P_0} a_{(i)}^j \qquad \bar{d}_k^{(i)}=\sum_j \left(\frac{\partial g^j}{\partial \bar{q}^k}\right)_{P_0} d_j^{(i)} \tag{2.19}$$

and the $a_{(i)}^j$ and $d_j^{(i)}$ satisfy the equations (2.11b), remembering that now $(M_{ij})_{P_0}$ and $(K_{ij})_{P_0}$ are, respectively, the mass tensor and the hessian, (2.17d), at the point P_0.

Under the transformation (2.19) the local Hamiltonian (2.16) and the Hamilton equations (2.18) can be written as

$$\bar{H}^L(\boldsymbol{\eta},\boldsymbol{\zeta})=(V)_{P_0}+\sum_i K_i\eta^i+\tfrac{1}{2}\sum_i(\zeta_i^2+\lambda_i\eta^{i2})+\ldots \tag{2.20}$$

$$\dot{\eta}^i=\zeta_i \qquad -\dot{\zeta}_i=K_i+\lambda_i\eta^i. \tag{2.21}$$

In these equations K_i is the component of the gradient vector field at P_0 in the direction of the ith local normal mode vector:

$$K_i=\sum_k\left(\frac{\partial V}{\partial q^k}\right)_{P_0} a_{(i)}^k. \tag{2.22}$$

The equations (2.20) and (2.21) show that the local normal modes are decoupled degrees of freedom at P_0. However, since the gradient vector field does not vanish at P_0, in general the pairs ζ_i, η^i, $i=0,\ldots,N-1$ are not invariant planes at P_0. A local normal mode defines an invariant plane at P_0 only if the gradient vector field at this point is in the direction of this normal mode. Denoting this maximally decoupled local degree of freedom by η^0, ζ_0, the above condition gives

$$K_i=\sum_k\left(\frac{\partial V}{\partial q^k}\right)_{P_0} a^k(i)=0 \qquad i\neq 0. \tag{2.23}$$

So a maximally decoupled local degree of freedom exists at the point P_0 only if the following equations are satisfied at this point:

$$\sum_{k,l} a_{(i)}^k(K_{kl})_{P_0}a_{(j)}^l=\lambda_i\,\delta_{ij} \tag{2.24a}$$

$$\sum_{k,l} a_{(i)}^k(M_{kl})_{P_0}a_{(j)}^l=\delta_{ij} \tag{2.24b}$$

$$\sum_k\left(\frac{\partial V}{\partial q^k}\right)_{P_0} a_{(i)}^{(k)}=0 \qquad i\neq 0. \tag{2.24c}$$

The first two equations define the local normal modes and the last one shows that the zeroth normal mode is maximally decoupled. These equations are the local harmonic approximation equations of Rowe and Bassermann (1976). To proceed in our discussion we can easily see that the equations (2.23) are satisfied once one has

$$\left(\frac{\partial V}{\partial q^k}\right)_{P_0} = (\text{grad } V)_{P_0} d_k^{(0)}. \tag{2.25}$$

From (2.24) and (2.11*b*) it follows that

$$\sum_{k,l} (K_{il})_{P_0} (B^{lj})_{P_0} \left(\frac{\partial V}{\partial q^j}\right)_{P_0} = \lambda_0 \left(\frac{\partial V}{\partial q^i}\right)_{P_0}. \tag{2.26}$$

Thus we can state that a maximally decoupled local degree of freedom exists only at the points where the gradient vector field is a local normal mode vector (Rowe 1982). It can be easily shown that the points in configuration space where this condition holds are the ones in which the variation of $|\text{grad } V|^2$ in an equipotential surface vanishes (Rowe and Ryman 1982). The curves which follow these points are called stationary paths (Rowe and Ryman 1982). Therefore we conclude that a maximally decoupled local degree of freedom exists only at points in a stationary path. Physically we are interested in the stationary path which is a valley of the potential (if it exists). In this case the stationary path is a minimal path which goes through the point of minimum of the potential and when we leave this point, λ_0 is the smallest proper frequency which becomes the only unstable one at large amplitudes. So the minimal curve is a valley if (Rowe and Ryman 1982)

$$\sum_{i,j} (X^i)_{P_0} (K_{ij})_{P_0} (X^j)_{P_0} > 0 \tag{2.27}$$

where $(\boldsymbol{X})_{P_0}$ is a vector perpendicular to the gradient field at a point P_0 in the minimal path:

$$\sum_i (X^i)_{P_0} \left(\frac{\partial V}{\partial q^i}\right)_{P_0} = 0. \tag{2.28}$$

Defining the equation of the valley path by $q^i = g^i(\eta^0)$, one has, using (2.26)

$$\sum_{k,l} (K_{il})_{\eta^0} (B^{lj})_{\eta^0} \left(\frac{\partial V}{\partial q^j}\right)_{\eta^0} = \lambda_0(\eta^0) \left(\frac{\partial V}{\partial q^i}\right)_{\eta^0} \tag{2.29}$$

where we have used the notation

$$(K_{il})_{\eta^0} \doteq K_{il}(\boldsymbol{g}(\eta_0)).$$

In configuration space, we consider a normal coordinate system (Synge and Schild 1969) such that one of the orthogonal trajectories is the valley path, $q^i = g^i(\eta^0)$ where η^0 is the arc length. In this case the equation of the two-dimensional surface in phase space is

$$q^i = g^i(\eta^0) \qquad p_i = \sum_l (M_{il})_{\eta^0} \frac{\partial g^l}{\partial \eta^0} \zeta_0. \tag{2.30}$$

In the LHA the optimal collective path is the valley path, the collective motion is the motion of the system constrained to the surface (2.30) generated by the valley path and the collective variables, the pair of canonical variables which span this surface, are η^0 and ζ_0.

3. Global maximal decoupling and the self-consistent collective coordinate method (SCC)

In the approach of Marumori and collaborators (Marumori *et al* 1980, Sakata *et al* 1983) the idea is to find a maximally decoupled subspace of the whole phase space. In the case of one collective degree of freedom this subpace is a two-dimensional phase space which defines an invariant surface in the whole phase space (Da Providência and Urbano 1982). By definition Σ is an invariant surface in phase space if, given that the system is initially in this surface, it remains on it. In other words there exist solutions of the Hamilton equations such that if $\boldsymbol{q}_0$ and $\boldsymbol{p}_0$ are in Σ, $\boldsymbol{q}(t)$ and $\boldsymbol{p}(t)$ remain on Σ, where $\boldsymbol{p}(t)$ and $\boldsymbol{q}(t)$ are solutions of the Hamilton equations with the initial conditions

$$\boldsymbol{q}(0)=\boldsymbol{q}_0, \qquad \boldsymbol{p}(0)=\boldsymbol{p}_0.$$

To establish the conditions which define the maximally decoupled subspace in our case, consider the point transformation:

$$\begin{aligned} &q^i=g^i(\boldsymbol{\eta}) && \eta^i=f^i(\boldsymbol{q}) \\ &p_i=\sum_k \frac{\partial f^k}{\partial q^i}\zeta_k && \zeta_i=\sum_x \frac{\partial g^k}{\partial \eta^i}p_k \\ &\sum_k \frac{\partial g^i}{\partial \eta^k}\frac{\partial f^k}{\partial q^j}=\delta^i j. \end{aligned} \tag{3.1}$$

Under (3.1) the Hamiltonian transforms to (equations (2.4) and (2.5)):

$$\begin{aligned} &\bar{K}(\boldsymbol{\zeta},\boldsymbol{\eta})=\tfrac{1}{2}\sum_{i,j}\bar{B}^{ij}(\boldsymbol{\eta})\zeta_i\zeta_j+\bar{V}(\boldsymbol{\eta}) \\ &\bar{B}^{ij}(\boldsymbol{\eta})=\sum_{m,n}\frac{\partial f^i}{\partial q^m}(\boldsymbol{g}(\boldsymbol{\eta}))\frac{\partial f^j}{\partial q^n}(\boldsymbol{g}(\boldsymbol{\eta}))B^{mn}(\boldsymbol{g}(\boldsymbol{\eta})) \\ &\bar{V}(\boldsymbol{\eta})=V(\boldsymbol{g}(\boldsymbol{\eta})). \end{aligned} \tag{3.2}$$

A two-dimensional subspace of the whole phase space is defined by the equations

$$\eta^i=\zeta_i=0 \qquad i\neq 0. \tag{3.3}$$

The equations (3.3) of the two-dimensional surface in phase space can be written as

$$q^i=(g^i)_{\eta^0}=g^i(\eta^0) \qquad i=0,\ldots,N-1 \tag{3.4a}$$

$$p^i=\left(\frac{\partial f^0}{\partial q^i}\right)_{\eta^0}\zeta_0 \tag{3.4b}$$

$$\sum_k\left(\frac{\partial g^k}{\partial \eta^j}\right)_{\eta^0}\left(\frac{\partial f^i}{\partial q^k}\right)_{\eta^0}=\delta^i j \tag{3.4c}$$

where we use the notation

$$\left(\frac{\partial f^0}{\partial q^i}\right)_{\eta^0}=\left(\frac{\partial f^0}{\partial q^i}\right)_{\eta=(\eta^0,0,\ldots,0)} \qquad \text{etc.}$$

Now the requirement that (3.3) is a maximally decoupled subspace imposes that

$$\left[\frac{\partial \bar{K}}{\partial \eta^i}\right]_{\eta^0,\zeta_0}=0 \qquad \left[\frac{\partial \bar{K}}{\partial \zeta_i}\right]_{\eta^0,\zeta_0}=0 \qquad i=1,\ldots,N-1 \tag{3.5}$$

where we use the notation

$$\left[\frac{\partial \bar{K}}{\partial \eta^i}\right]_{\eta^0,\zeta_0} = \left[\frac{\partial \bar{K}}{\partial \eta^i}\right]_{\substack{\boldsymbol{\zeta}=(\zeta_0,0,\ldots,0)\\ \boldsymbol{\eta}=(\eta^0,0,\ldots,0)}}.$$

Furthermore, the evolution of the system in the maximally decoupled subspace is given by

$$\dot{\eta}^0 = \left[\frac{\partial \bar{K}}{\partial \zeta_0}\right]_{\eta^0,\zeta_0} \qquad -\dot{\zeta}_0 = \left[\frac{\partial \bar{K}}{\partial \eta^0}\right]_{\eta^0,\zeta_0}. \tag{3.6}$$

The equations (3.5) are the Marumori equations of the maximally decoupled subspace (Sakata *et al* 1983). Given (3.2) these equations can be rewritten as

$$(\bar{B}^{i0})_{\eta^0} = 0 \qquad i \neq 0 \tag{3.7a}$$

$$\left(\frac{\partial \bar{V}}{\partial \eta^i}\right)_{\eta^0} = 0 \qquad i \neq 0 \tag{3.7b}$$

$$\left(\frac{\partial \bar{B}^{00}}{\partial \eta^i}\right)_{\eta^0} = 0 \qquad i \neq 0. \tag{3.7c}$$

The equations (3.7) are easily seen to be equal to Villars equations (I), (II) and (III), respectively (Villars 1977). To establish the geometrical properties of the maximally decoupled subspace we use the equations (3.2) and (3.4) to write equations (3.7) as

$$\sum_m \left(\frac{\partial V}{\partial q^m}\right)_{\eta^0} \left(\frac{\partial g^m}{\partial \eta^i}\right)_{\eta^0} = 0 \qquad i \neq 0 \tag{3.8a}$$

$$\frac{\partial g^j}{\partial \eta^0} = \frac{1}{(\text{grad } V)_{\eta^0}} \sum_m (B^{jm})_{\eta^0} \left(\frac{\partial V}{\partial q^m}\right)_{\eta^0} \tag{3.8b}$$

$$\frac{\partial^2 g^j}{\partial \eta^{0^2}} + \sum_{m,n} \left(\left\{ {j \atop mn} \right\}\right)_{\eta^0} \frac{\partial g^m}{\partial \eta^0} \frac{\partial g^n}{\partial \eta^0} = 0 \tag{3.8c}$$

where we set the scale such that η^0 is the arc length along the curve $q^i = g^i(\eta^0)$. The equations (3.8*b*) show that the curve $q^i = g^i(\eta^0)$ is a gradient line and the equation (3.8*c*) that it is a geodesic line. Therefore the curve (3.4*a*) is a geodesic gradient line (in a manifold whose metric tensor is the mass tensor). The equations (3.8*a*) only impose that the coordinate lines $\eta^i(\eta^j = \text{constant}, j \neq i)$, $i \neq 0$, cross the geodesic gradient line perpendicularly and a coordinate system with this property always exists (Synge and Schild 1969). What we have just shown tells us that a maximally decoupled subspace (when it exists) is such that the curve $q^i = g^i(\eta^0)$ is a geodesic gradient line. However, from a physical point of view, not all maximally decoupled subspaces are of interest. We should add the boundary condition that near the minimum the surface should coincide with the plane of the lowest frequency normal mode. Besides, only the stable ones should be considered. To see what that means, suppose that the two-dimensional subspace (3.4) is maximally decoupled. The pair of canonical variables η^0, ζ_0 which span this subspace will be identified with the collective degree of freedom and the other pairs of canonical variables, η^i, ζ_i, $i = 1, \ldots, N-1$, with the non-collective ones. The stability condition of a maximally decoupled subspace depends on the coupling properties of the collective and non-collective degrees of freedom. To study this coupling let us expand the Hamiltonian (3.2) to second order in the non-collective degrees of freedom (Sakata *et al* 1983):

$$\bar{K}(\boldsymbol{\eta}, \boldsymbol{\zeta}) = H_{\text{coll}}(\eta^0, \zeta_0) + \frac{1}{2} \sum_{i,j\neq 0} \left(\left[\frac{\partial^2 \bar{K}}{\partial \zeta_i \zeta_j}\right]_{\eta^0, \zeta_0} \zeta_i \zeta_j + \left[\frac{\partial^2 \bar{K}}{\partial \eta^i \, \partial \eta^j}\right]_{\eta^0, \zeta_0} \eta^i \eta^j + 2\left[\frac{\partial^2 \bar{K}}{\partial \zeta_i \, \partial \eta^j}\right]_{\eta^0, \zeta_0} \zeta_i \eta^j \right) + \ldots \tag{3.9}$$

where

$$H_{\text{coll}}(\eta^0, \zeta_0) = [K(\boldsymbol{\eta}, \boldsymbol{\zeta})]_{\eta^0, \zeta_0} = \tfrac{1}{2}(\bar{B}^{00})_{\eta^0} \zeta_0^2 + (\bar{V})_{\eta^0}$$

$$(\bar{B}^{00})_{\eta^0} = 1 \tag{3.10}$$

$$(\bar{V})_{\eta^0} = V(\boldsymbol{g}(\eta^0)) = V_{\text{coll}}(\eta^0)$$

$$\left[\frac{\partial^2 K}{\partial \zeta_i \zeta_j}\right]_{\eta^0, \zeta_0} = (\bar{B}^{ij})_{\eta^0} \tag{3.11}$$

$$\left[\frac{\partial^2 \bar{K}}{\partial \eta^i \, \partial \eta^j}\right]_{\eta^0, \zeta_0} = \left(\frac{\partial^2 \bar{V}}{\partial \eta^i \, \partial \eta^j}\right)_{\eta^0} + \left(\frac{\partial^2 \bar{B}^{00}}{\partial \eta^i \, \partial \eta^j}\right)_{\eta^0} \zeta_0^2 \tag{3.12}$$

$$\left[\frac{\partial^2 \bar{K}}{\partial \zeta_i \, \partial \eta^j}\right]_{\eta^0, \zeta_0} = \left(\frac{\partial \bar{B}^{i0}}{\partial \eta^j}\right)_{\eta^0} \zeta_0^2 \tag{3.13}$$

where $i, j \neq 0$. The equations of motion for the non-collective degrees of freedom, to first order in these variables, are given by

$$\dot{\eta}^i(t) = \sum_{j=1}^{N-1} \left[\frac{\partial^2 \bar{K}}{\partial \zeta_i \, \partial \zeta_j}\right]_{\substack{\eta^0 = \eta^0(t) \\ \zeta_0 = \zeta_0(t)}} \zeta_j + \left[\frac{\partial^2 \bar{K}}{\partial \zeta_i \, \partial \eta^j}\right]_{\substack{\eta^0 = \eta^0(t) \\ \zeta_0 = \zeta_0(t)}} \eta^j \tag{3.14}$$

$$-\dot{\zeta}_i(t) = \sum_{j=1}^{N-1} \left[\frac{\partial^2 \bar{K}}{\partial \eta^i \, \partial \zeta_j}\right]_{\substack{\eta^0 = \eta^0(t) \\ \zeta_0 = \zeta_0(t)}} \zeta_j + \left[\frac{\partial^2 \bar{K}}{\partial \eta^i \, \partial \eta^j}\right]_{\substack{\eta^0 = \eta^0(t) \\ \zeta_0 = \zeta_0(t)}} \eta^j \tag{3.15}$$

where $\eta^0(t)$ and $\zeta_0(t)$ are the solutions of the Hamilton equations constrained to the maximally decoupled subspace (3.6):

$$\dot{\eta}^0(t) = \zeta_0(t) \qquad \dot{\zeta}_0(t) = -(\partial V_{\text{coll}}/\partial \eta^0)(\eta^0).$$

A maximally decoupled subspace is stable if, given that $\zeta_i(t)|_{t=0}$ and $\eta^i(t)|_{t=0}$, $i \neq 0$, is small, then $\zeta_i(t)$ and $\eta^i(t)$ remain small, where $\zeta_i(t)$ and $\eta^i(t)$ are solutions of the equations (3.15).

Finally notice that the equation (3.9) gives another criterion to identify a maximally decoupled subspace: the coupling of the collective variables and the non-collective ones is at least second order in these last variables.

4. Global maximal decoupling versus local maximal decoupling

The discussion in § 2 has shown that one can find a maximally decoupled local degree of freedom only at points in a stationary path. Furthermore, physical considerations indicate that a collective path should be associated with a minimal path which is a valley. However in general these curves are not integral curves of the potential gradient field (it is not a gradient line) as can be seen in figure 2 of Rowe and Ryman (1982).

To see this note that at each point in the stationary path we can define the normal mode vectors, the potential gradient vector and the tangent vector to the stationary path. As this path is a stationary path, the potential gradient is in the direction of one of the normal modes. However, in general, the tangent vector is not in the direction of the potential gradient. A consequence of this fact is that motion along a stationary path is not motion along a maximally decoupled local degree of freedom. On the other hand, when the stationary path is a gradient line, at each point on it the tangent is in the direction of the maximally decoupled local degree of freedom. In this case motion along a stationary path is motion along a maximally decoupled local degree of freedom.

To see under what conditions this is accomplished consider the equation of the stationary path $q^i = g^i(\eta^0)$, where η^0 is the arc length of the curve. Imposing that the stationary path be also a gradient line, $g^i(\eta^0)$ should obey the equations

$$\frac{\mathrm{d}g^i}{\mathrm{d}\eta^0}=\frac{1}{(\operatorname{grad} V)_{\eta^0}}\sum_j (B^{ij})_{\eta^0}\left(\frac{\partial V}{\partial q^j}\right)_{\eta^0}, \tag{4.1}$$

besides equations (2.29).

However (2.29) and (4.1) leads to

$$\frac{\mathrm{d}^2g^i}{\mathrm{d}\eta^{0^2}}+\sum_{mj}\left(\left\{ {i \atop mj} \right\}\right)_{\eta^0}\frac{\partial g^m}{\partial\eta^0}\frac{\partial g^j}{\partial\eta^0}=0 \tag{4.2}$$

which is the equation of a geodesic in a manifold whose metric tensor is the mass tensor. In this case the stationary path is necessarily a geodesic line and so, a geodesic gradient line. When this condition is satisfied the two approaches are equivalent. Therefore, the requirement that motion along a stationary path be motion along a maximally decoupled local degree of freedom is satisfied only if the stationary path defines a maximally decoupled global degree of freedom.

5. Conclusions

Many proposals of 'optimal' collective paths have appeared in the literature. The geometrical properties of three of the proposals turn out to be natural (de Passos 1982) once one notices that the potential gradient and the local normal modes are vector fields in the configuration space *C*. The 'optimal' path of Villars (Villars 1977, Goeke and Reinhard 1978) is an integral curve of the potential gradient field and the one of Moya de Guerra (Moya de Guerra and Villars 1977) is an integral curve of the normal mode field. The points where these two vector fields are parallel define the LHA 'optimal' path (Rowe and Bassermann 1976, Rowe 1982). In general these requirements do not select a unique path (Goeke *et al* 1981). The Villars path is not uniquely defined since a gradient line goes through every point. Furthermore, the lowest frequency normal mode at the potential minimum cannot be used to select one particular gradient line since, at this point, all gradient lines are tangent to it (Rowe 1982). However when the potential energy surface has a saddle point it was suggested to adopt the gradient line from the saddle point to the minimum as the 'optimal path' (Goeke *et al* 1981). In the case of the Moya de Guerra path one selects the integral curve of the lowest frequency normal mode, which goes through the point of minimum. In the LHA one selects the minimal valley path as the 'optimal' collective path. On the other hand, the 'optimal' path of the SCC method (Marumori *et al* 1980, Sakata *et al* 1983) define an invariant two-dimensional subspace of the whole phase space. In this paper we investigate in detail two proposals of 'optimal' path, one based on the LHA and the other on the SCC method. This is done in the framework of classical mechanics. The fundamental point in our derivation of the LHA is the concept of local maximal decoupling. A careful study of its physical meaning shows that it depends on an *a priori* choice of a metric connection in the configuration space manifold. Each choice will give rise to different decoupling requirements and, as a consequence, different 'optimal' paths. In our case the choice is naturally dictated by the dynamics and it is the metric connection induced by the mass tensor. Once this choice is made we show how to derive the equations of the optimal path by imposing that at each point on it there exists a maximally decoupled local degree of freedom. The points where this condition is satisfied are such that the gradient vector field is in the direction of a local normal mode in a manifold whose metric tensor is the mass tensor. It is also shown that the curves which follow these points are stationary curves. On the other hand, in the SCC method one tries to find a maximally decoupled subspace of the whole phase space. This subspace defines an invariant surface in phase space and in our case it is the surface generated by a geodesic gradient line in the configuration space. Thus one sees that in the SCC method one requires a global maximal decoupling. When this condition is satisfied the invariant surface is an example of a Baranger-Veneroni (1978) spaghetto. From our discussion it is clear that the condition of local maximal decoupling is always satisfied but not that of global maximal decoupling. The difference stems from the fact that, in general, motion along a stationary path is not motion along a maximally decoupled local degree of freedom. When we investigate under what conditions motion along a stationary path is motion along a maximally decoupled local degree of freedom, one sees that this happens only if this curve is also a gradient line, in which case it becomes a geodesic gradient line. In this case the stationary path defines an invariant two-dimensional subspace of the whole phase space and the 'optimal' paths of the LHA and SCC methods coincide. Furthermore, one sees, by what we said above, that this curve is also a Villars path (it is a gradient line) and a Moya de Guerra path (it is an integral curve of the normal mode field since it is a stationary path which is a gradient line).

References

Baranger M and Veneroni M 1978 *Ann. Phys., NY* **114** 123-200

Da Providência J and Urbano J N 1982 *Lecture Notes in Physics* **171** 343-9

de Passos E J V 1982 *Lecture Notes in Physics* **171** 350-7

Goeke K and Reinhard P G 1978 *Ann. Phys., NY* **112** 328-55

Goeke K, Reinhard P G and Grummer F 1983 *Ann. Phys., NY* **150** 504-51

Goeke K, Reinhard P G and Rowe D J 1981 *Nucl. Phys.* A **359** 408-30

Marumori T, Maskawa T, Sakata F and Kuriyama A 1980 *Prog. Theor. Phys.* **64** 1294-314

Moya de Guerra E and Villars F 1977 *Nucl. Phys.* A **285** 297-316

Rowe D J 1982 *Nucl. Phys.* A **391** 307-26

Rowe D J and Bassermann R 1976 *Can. J. Phys.* **54** 1941-68

Rowe D J and Ryman A 1982 *J. Math. Phys.* **23** 732-5

Rowe D J, Ryman A and Rosensteel G 1980 *Phys. Rev.* C **22** 2362-73

Sakata F, Hashimoto Y, Marumori T and Une T 1983 *Prog. Theor. Phys.* **70** 424-38

Synge J L and Schild A 1969 *Tensor Calculus* (Toronto: University of Toronto Press)

Villars F 1977 *Nucl. Phys.* A **285** 269-96