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THE CONCEPT OF "OPTIMAL" PATH IN CLASSICAL MECHANICS

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ABSTRACT

In this work 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 allow us to establish the conditions under which they become equivalent.

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I. INTRODUCTION

In a series of papers many authors (Rowe 1976, Rowe 1982, Marumori 1980, Sakata 1983, Villars 1977) proposed self-consistent theories of large amplitude collective motion. The starting point of all these developments is the Time-dependent Hartree-Fock theory (TDHF) and therefore they are semiclassical in character. This makes it possible to cast all these theories in a classical language and we confine all discussion in this paper to the case where the corresponding classical Hamiltonian is at most quadratic in the momenta. 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 1976, Rowe 1982) one determines the "optimal" path by requiring that, at each point on it, there exist a maximally decoupled local degree of freedom. On the other hand, in the self-consistent collective coordinate method (SCC), (Marumori 1980, Sakata 1983) one imposes that the "optimal" path define a maximally decoupled subspace of the whole phase space. This maximally decoupled subspace is an invariant two-dimensional surface in phase space (Da Providência and Urbano 1982, Sakata 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 1983). In despite of this, many points deserve further clarifications. The ones which we believe to be the most importants are: i) a better understanding of the concept of local maximal decoupling, 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 section II 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. Our discussion shows clearly that, to be well defined, this concept depends on an à priori choice of a metric connection in the configuration space manifold. In section III we present our derivation of the SCC method based on the concept of global maximal decoupling. In section IV we discuss in what respect these two approaches differ and establish the conditions under which they become equivalent. In section V 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, give 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.

II. 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 $q = (q^0, q^1, \dots, q^{N-1})$ are the local coordinates of a point C and $p = (p_0, p_1, \dots, p_{N-1})$ the components of a co-vector at this point, the 2N numbers $q = (q^0, q^1, \dots, q^{N-1})$

and $p = (p_0, \dots, p_{N-1})$ are the canonical coordinates in T^*C. The N numbers $\underset{\sim}{p}$ are the momenta associated to the N coordinates $\underset{\sim}{q}$.

The canonical transformations which preserve the cotangent bundle structure of C are the point transformations, defined by:

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

and its inverse

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

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

These transformations, eqs. (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

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

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

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

where

$$\bar{V}(\bar{q}) = V(q(\bar{q}))$$

$$\bar{B}^{ij}(\bar{q}) = \sum_{k,\ell} \frac{\partial f^i}{\partial q^\ell}(q(\bar{q}))\ \frac{\partial f^j}{\partial q^k}(q(\bar{q}))\ B^{k\ell}(q(\bar{q})) \quad . \tag{2.5}$$

The equations (2.1) and (2.5) show that, by a change of coordinates, the potential $V(q)$ transforms as a scalar, the $B^{ij}(q)$ transform as the contravariant components of a tensor, the mass tensor, and the momenta transform as the components of a co-vector.

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

$$\dot{q}^i = \sum_k B^{ik}(q)\ p_k$$

$$\ddot{q}^i + \sum_{j,k} \left\{ {i \atop j\ k} \right\} \dot{q}^j\ \dot{q}^k = - \sum_j B^{ij} \frac{\partial V}{\partial q^j} \tag{2.6}$$

In equation (2.6) $\left\{ {i \atop j\ k} \right\}$ are the components of the metric connection (Christoffel symbols) induced by the mass tensor M_{ij} (Synge and Schild 1969):

$$\left\{ {i \atop j\ k} \right\} = \sum_\ell B^{i\ell}(q)\ \frac{1}{2} \left\{ \frac{\partial M_{\ell j}(q)}{\partial q^k} + \frac{\partial M_{\ell k}(q)}{\partial q^j} - \frac{\partial M_{jk}(q)}{\partial q^\ell} \right\}$$

$$\sum_\ell B^{i\ell}(q)\ M_{\ell k}(q) = \delta^i{}_k \quad . \tag{2.7}$$

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.

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:

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

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

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

where

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

$$\beta_i = p_i \quad ,$$

q and p being the coordinates and the momenta of a point in the neighbourhood of P_0. In eq. (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,

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

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

$$(K_{ij})_{P_0} = \left[\frac{\partial^2 V}{\partial q^i \partial q^j}(\underset{\sim}{q})\right]_{\underset{\sim}{q}=(\underset{\sim}{q})_{P_0}} \quad . \tag{2.9-c}$$

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

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

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

$$\begin{aligned} \zeta_i &= \sum_k a^k_{(i)} \beta_k \\ \eta^i &= \sum_k d^{(i)}_k \alpha^k \end{aligned} \tag{2.11-a}$$

if

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

In eqs. (2.11) $\hat{A}^T$ 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 $a^k_{(i)}$, $k = 0,\dots,N-1$ (i fixed) are the contravariant components of a vector at the point P_0, which is the i^{th} local normal mode vector. Using the transformation (2.11), the Hamiltonian and the Hamilton equations near P_0 are given by:

$$\overline{H}^L(\underset{\sim}{\zeta},\underset{\sim}{\eta}) = (V)_{P_0} + \frac{1}{2}\sum_i (\zeta_i^2 + \lambda_i \eta^{i2}) + \dots \tag{2.12}$$

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

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 $i = 0,\dots,N-1$ defines, at the point P_0, an invariant plane in phase space. $\sum_{P_0}$ is an invariant plane at the point P_0 if, given that $\underset{\sim}{\alpha}_0, \underset{\sim}{\beta}_0$ is a point in this plane, $\underset{\sim}{\alpha}(t)$, $\underset{\sim}{\beta}(t)$ remains on it, where $\underset{\sim}{\alpha}(t)$, $\underset{\sim}{\beta}(t)$ are solutions of the Hamilton equations (2.10) with the initial condition $\underset{\sim}{\alpha}_0 = \underset{\sim}{\alpha}(t)\big|_{t=0}$, $\underset{\sim}{\beta}_0 = \underset{\sim}{\beta}(t)\big|_{t=0}$. 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 covariant derivative is equal to 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, à priori, a metric connection. In our case the natural choice is the metric connection induced by the mass tensor, eq. (2.7).

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

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

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

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

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

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

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

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

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

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

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

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

The equations (2.17) deserve several comments. Firstly equation (2.17-d) shows that the generalization 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, eq. (2.16). This term depends on the potential gradient field at P_0, as expected. Finally we see that a different choice of the metric connection will change only the definition of the local elastic tensor, the mass tensor and the potential gradient field being the same. Given (2.16), the Hamilton equations near P_0 can be written as:

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

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

$$\eta^i = \sum_k \bar{d}_k^{(i)}\, \bar{\alpha}^k$$

$$\zeta_i = \sum_k \bar{a}^k_{(i)}\, \bar{\beta}_k$$

if

$$\begin{aligned} \bar{a}^k_{(i)} &= \sum_j \left(\frac{\partial f^k}{\partial q^j}\right)_{P_0} a^j_{(i)} \\ \bar{d}_k^{(i)} &= \sum_j \left(\frac{\partial g^j}{\partial \bar{q}^k}\right)_{P_0} d_j^{(i)} \end{aligned} \tag{2.19}$$

and the $a^j_{(i)}$ and $d_j^{(i)}$ satisfy the equations (2.11-b),

remembering that now $(M_{ij})_{P_0}$ and $(K_{ij})_{P_0}$ are, respectively, the mass tensor and the hessian, eq. (2.17-d), 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:

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

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

In these equations K_i is the component of the gradient vector field at P_0 in the direction of the i^{th} local normal mode vector:

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

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

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

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

$$\sum_{k,\ell} a^k_{(i)} (K_{k\ell})_{P_0} a^\ell_{(j)} = \lambda_i \delta_{ij} \tag{2.24-a}$$

$$\sum_{k,\ell} a^k_{(i)} (M_{k\ell})_{P_0} a^\ell_{(j)} = \delta_{ij} \tag{2.24-b}$$

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

The first two equations define the local normal modes and the last one shows that the 0^{th} normal mode is maximally decoupled. These equations are the local harmonic approximation equations of Rowe and Bassermann (Rowe 1982). To proceed in our discussion we can easily see that the equations (2.23) are satisfied once one has:

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

From eqs. (2.24) and (2.11-b) it follows:

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

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 (Rowe and Ryman 1982):

$$\delta_{\mid} \text{grad } V|^2 = 0 \quad ,$$

in an equipotential surface. The curves which follow these points are called stationary curves (Rowe and Ryman 1982). Therefore we conclude that a maximally decoupled local degree of freedom exists only at points in a stationary curve. Physically we are interested in the stationary curve which is the valley of the potential (if it exists). In this case the stationary curve is a minimal curve 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 minimum 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 $(X^i)_{P_0}$ is a vector perpendicular to the gradient field at a point P_0 in the stationary curve:

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

Defining the equation of a stationary path by $q^i = g^i(\eta^0)$, one has, using eqs. (2.26):

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

where we used the notation

$$(K_{i\ell})_{\eta^0} = K_{i\ell}(\underset{\sim}{g}(\eta_0)) \quad .$$

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

$$q^i = g^i(\eta^0) \qquad p_i = \sum_{\ell} (M_{i\ell})_{\eta^0} \frac{\partial g^\ell}{\partial \eta^0} \zeta_0 \tag{2.30}$$

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

III. GLOBAL MAXIMAL DECOUPLING AND THE SELF-CONSISTENT COLLECTIVE COORDINATE METHOD (SCC)

In the approach of Marumori and collaborators (Marumori 1980, Sakata 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 subspace is a two-dimensional phase space which defines an invariant surface in the whole phase space (Da Providência and Urbano 1982). By definition $\sum$ 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 q_0 and p_0 are in $\sum$, $\underset{\sim}{q}(t)$ and $\underset{\sim}{p}(t)$ remain on $\sum$, where $\underset{\sim}{p}(t)$ and $\underset{\sim}{q}(t)$ are solutions of

the Hamilton equations with the initial conditions

$$\underset{\sim}{q}(0) = \underset{\sim}{q}_0 \quad , \quad \underset{\sim}{p}(0) = \underset{\sim}{p}_0 \quad .$$

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

$$q^i = g^i(\underset{\sim}{\eta}) \qquad \eta^i = f^i(\underset{\sim}{q})$$

$$p_i = \sum_k \frac{\partial f^k}{\partial q^i} \zeta_k \qquad \zeta_i = \sum_k \frac{\partial g^k}{\partial \eta^i} p_k \tag{3.1}$$

$$\sum_k \frac{\partial g^i}{\partial \eta^k} \frac{\partial f^k}{\partial q^j} = \delta^i{}_j$$

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

$$\bar{K}(\underset{\sim}{\zeta},\underset{\sim}{\eta}) = \frac{1}{2} \sum_{i,j} \bar{B}^{ij}(\underset{\sim}{\eta})\, \zeta_i \zeta_j + \bar{V}(\underset{\sim}{\eta})$$

$$\bar{B}^{ij}(\underset{\sim}{\eta}) = \sum_{m,n} \frac{\partial f^i}{\partial q^m}(\underset{\sim}{g}(\underset{\sim}{\eta})) \frac{\partial f^j}{\partial q^n}(\underset{\sim}{g}(\underset{\sim}{\eta}))\, B^{mn}(\underset{\sim}{g}(\underset{\sim}{\eta})) \tag{3.2}$$

$$\bar{V}(\underset{\sim}{\eta}) = V(\underset{\sim}{g}(\underset{\sim}{\eta}))$$

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

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

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

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

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

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

where we use the notation

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

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

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

where we use the notation,

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

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

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

The equations (3.5) are the Marumori equations of the maximal decoupled subspace (Sakata 1983). Given (3.2)

these equations can be rewritten as:

$$(\overline{B}^{i0})_{\eta^0} = 0 \qquad i \neq 0 \qquad (3.7\text{-a})$$

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

$$\left(\frac{\partial \overline{B}^{00}}{\partial \eta^i}\right)_{\eta^0} = 0 \qquad i \neq 0 \qquad (3.7\text{-c})$$

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:

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

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

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

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 η^i (η^j = cte $j \neq i$), $i \neq 0$, 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 eq. (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, $i = 1,\dots,N-1$, 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 1983):

$$\overline{K}(\underline{\eta},\underline{\zeta}) = H_{coll}(\eta^0,\zeta_0) + \frac{1}{2}\sum_{i,j\neq 0}\left\{\left[\frac{\partial^2\overline{K}}{\partial\zeta_i\zeta_j}\right]_{\eta^0,\zeta_0}\zeta_i\zeta_j + \left[\frac{\partial^2\overline{K}}{\partial\eta^i\partial\eta^j}\right]_{\eta^0,\zeta_0}\eta^i\eta^j + 2\left[\frac{\partial^2\overline{K}}{\partial\zeta_i\partial\eta^j}\right]_{\eta^0,\zeta_0}\zeta_i\eta^j\right\} + \dots \qquad (3.9)$$

where

$$H_{coll}(\eta^0,\zeta_0) = [K(\underline{\eta},\underline{\zeta})]_{\eta^0,\zeta_0} = \frac{1}{2}(\overline{B}^{00})_{\eta^0}\,\zeta_0^2 + (\overline{V})_{\eta^0}$$

$$(\overline{B}^{00})_{\eta^0} = 1 \qquad (3.10)$$

$$(\overline{V})_{\eta^0} = V(\underline{g}(\eta^0)) = V_{coll}(\eta^0)$$

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

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

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

The equations of motion for the non-collective degrees of freedom, to first order in these variables, are given by:

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

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

where $\eta^0(t)$ and $\zeta_0(t)$ are the solutions of the Hamilton equations constrained to the maximally decoupled sub-space, eqs. (3.6):

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

A maximally decoupled subspace is stable if, given that $\zeta_i(t)\big|_{t=0}$ and $\eta^i(t)\big|_{t=0}$ $i \neq 0$ 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 other 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.

IV. GLOBAL MAXIMAL DECOUPLING VERSUS LOCAL MAXIMAL DECOUPLING

The discussion in section II has shown that one can find a maximally decoupled local degree of freedom only at points in a stationary path. However, in general, these curves are not integral curves of the potential gradient field (it is not a fall line), as can be seen in Fig. 2 of Rowe and Ryman (1982). A consequence of this fact is that different degrees of freedom are maximally decoupled at each point in a stationary path. To see this, note that at each point in a stationary path, the potential gradient field points in the direction of the maximally decoupled local degree of freedom. However, since in general a stationary path is not a fall line, there is no coordinate line tangent to these vectors. On the other hand, when the stationary path is a fall line, at each point on it, the tangent is in the direction of the maximally decoupled local degree of freedom. In this case the same degree of freedom is maximally decoupled along it.

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 fall line, $g^i(\eta^0)$ should obey the equations:

$$\frac{dg^i}{d\eta^0} = \frac{1}{(\text{grad } V)_{\eta^0}} \sum_j (B^{ij})_{\eta^0} \left(\frac{\partial V}{\partial q^j}\right)_{\eta^0} , \qquad (4.1)$$

besides equations (2.29).

However (2.29) and (4.1) leads to:

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

which is the equation of a geodesic in a manifold whose metric tensor is the mass tensor. Thus we see that the same degree of freedom is maximally decoupled at each point in a stationary path only if this path is a fall line. 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.

V. CONCLUSIONS

Schematically, two proposals of "optimal" paths appeared in the literature: one based on the LHA, the other on the SCC method. In this paper we investigate the significance of the concept of "optimal" path 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 à priori choice of a metric connection in the configuration space manifold. Each choice will give rise to different decoupling requirements and, by consequence, different "optimal" paths. In our case we argue that the natural choice 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 exist 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 spaghetto (Baranger 1978). 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, different degrees of freedom are maximally decoupled at each point in a stationary curve (the "optimal" path of the LHA). When we investigate under what conditions the same degree of freedom is maximally decoupled at each point in a stationary curve 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 two optimal paths coincide.

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