Determination of the collective Hamiltonian in a self-consistent theory of large amplitude adiabatic motion

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The starting point for most studies of large amplitude collective motion in nuclear physics, the time-dependent Hartree-Fock equations, can be mapped to a problem in classical Hamiltonian mechanics, which is the form of the problem studied in this work. For a system with N degrees of freedom, collective motion is identified with motion completely confined to a surface in $K<N$ dimensions. Conditions for the existence of such decoupled surfaces are worked out and a procedure for constructing them is formulated. For most practical problems, where such surfaces do not strictly exist, a concept of approximate decoupling is developed and a test of its accuracy is described. Our results generalize the method of maximum global decoupling found in the earlier literature.

I. INTRODUCTION

The aim of the theory of large amplitude collective motion is to decouple from a many-particle Hamiltonian a collective Hamiltonian expressed in terms of a few coordinates q^i, $i=1\ldots K$ and their conjugate momenta p_i. Confining our attention to the adiabatic limit and without worrying about operator ordering, this Hamiltonian has the form [$\underline{q}=(q^1\ldots q^K)$, etc.]

$$\bar{H}(\underline{q},\underline{p})=\tfrac{1}{2}p_i\bar{B}^{ij}(\underline{q})p_j+\bar{V}(\underline{q}) , \quad (1.1)$$

and is therefore characterized by a potential energy "surface" $\bar{V}(\underline{q})$ and a (reciprocal) mass matrix $\bar{B}^{ij}(\underline{q})$ which also plays a role as metric tensor. These are the "collective parameters" of this theory. Because of the restriction to quadratic terms in the momenta, (1,1) is supposed to describe low energy bound or continuum motion. During the past 15 years many contributions have been made to this subject. We cite some papers[1–32] which have had an impact, directly or indirectly on the present paper. Additional works by the same authors may be traced from the given references.

From some of this work[14,19,23,24,28,29] it has emerged that the collective parameters may be computed by considering a problem in classical Hamiltonian mechanics. For example, in the problem of nuclear physics, the usual starting point is time-dependent Hartree-Fock theory (THDF) which is recognized as a classical limit of the Fermion many-body problem. By a suitable change of variables, these equations may be shown to be of the classical Hamiltonian form, where the role of Hamiltonian is played by the Hartree-Fock energy functional. In general, this Hamiltonian is not quadratic in the momenta, but we have shown[28] how to carry out an expansion in powers of the momenta and thus arrive at a starting point, which is a classical Hamiltonian of the form

$$H=\tfrac{1}{2}\pi_\alpha B^{\alpha\beta}(\underline{\xi})\pi_\beta+V(\underline{\xi}) , \quad (1.2)$$

where $\underline{\xi}=(\xi^1\ldots\xi^N)$, $\underline{\pi}=(\pi_1\ldots\pi_N)$ are given canonical variables. In the nuclear problem, N may even go to infinity, but in any event we have a common starting point for problems, nuclear and non-nuclear. If the approach to the classical limit was done in a systematic way starting from a suitable quantum theory—generator coordinates,[11] equations of motion,[8,26,27] a Born-Oppenheimer method,[30] or a generalized coherent state method[7,9]—then quantum corrections may be included. The problem of "requantization" is dealt with in these works, and will not form a part of our presentation.

Given the Hamiltonian H of (1.2), the problem is then to decompose it into a sum of two parts

$$H=\bar{H}+\tilde{H} , \quad (1.3)$$

where $\bar{H}$ is the collective part (1.1) and $\tilde{H}$ depends on the collective coordinates as weakly as possible. The main question is: What is the best possible way of making this decomposition? In this paper, we shall develop a method, which we have termed the generalized valley approximation (GVA) which generalizes one of the methods developed previously in the literature, the method of maximum global decoupling.[7,17,20,22,23] Here it turns out that the application to more than one collective coordinate requires ideas not found in the previous literature.

A second approach, the local harmonic approximation (LHA) which is the vintage method[2] in this field, is in principle also applicable to any number of collective coordinates. This is a potentially important method which has been treated[23] as distinct from the predecessors of GVA. Since the technical content of this paper is already rather dense, we have reserved the analysis of the connection between GVA and LHA for a separate paper.

A third method, that of Goeke and Reinhard,[10,15,16] requires special mention because it is the only method that has been developed in practice to a point where it has been applied—very profitably—to a range of collision problems which involve one collective coordinate. Ironically, this is the only one of the methods which, by its special character, cannot be extended to more than one degree of freedom. However, if we are to achieve a fundamental understanding of the problem of low energy collective motion in the deformed region, we shall need to have a method applicable to more than one collective coordinate which is both theoretically sound and practical. In the present work we shall deal largely with the first requirement. It will be the burden of future work, starting with an accompanying paper, to show how to use the new method.

We turn to a consideration of the meaning of the decomposition (1.3), which is fundamental to our endeavors. To study this question, we carry out a point canonical transformation from the starting coordinates ξ^α to a new set q^μ. Of the latter, a subset q^i, $i=1,\ldots,K<N$ are deemed collective when they are appropriate descriptions of a family of *classically decoupled motions,* defined as follows: Let Σ be a K-dimensional surface parametrized by the new coordinates q^i. Let the system point be initially on Σ and let the initial velocity be along $T\Sigma$, the tangent plane to Σ. A motion is decoupled provided the system point remains on Σ in consequence of the action of the full Hamiltonian (1.2). On Σ the latter takes the values $\bar{H}(q^1,\ldots,q^K,p_1,\ldots,p_K)$. We may say that for $a=K+1,\ldots,N$, Σ is defined by the specification $p_a=0$ and (by definition) $q_a=0$. The goal is to find Σ and $\bar{H}$. This is the specific problem addressed in the body of our paper, where a solution is proposed.

As we shall come to understand, an exactly decoupled classical motion does not necessarily imply a well decoupled quantum motion. The decoupled classical motion generally takes place in a K-dimensional valley of the potential energy function V. There remains the question of how steeply the potential energy function climbs in directions orthogonal to the collective manifold Σ. Here the traditional criterion appears to be appropriate: A good measure should be the frequency of small oscillations of the noncollective degrees of freedom. This is not a completely trivial matter, however, since these frequencies are dependent on the coordinates of Σ. This problem is not discussed in the current work, but an example is given in the following paper.

The conditions which determine a decoupled classical motion are formulated in terms of Hamilton's equations of motion in Sec. II. Two equivalent sets are obtained, which are used interchangeably in whole or in part in the remainder of the development. The conditions are also seen to be derivable from variational arguments. In physical terms, since the manifold Σ may have intrinsic curvature, the essential conditions for decoupling are the absence of forces either "real" or of geometrical origin (centrifugal forces) normal to Σ. When there are constants of the motion in addition to the energy, these conclusions must be modified. In that event, decoupled motion may occur partially or (in extreme cases) totally in consequence of a balance of the two types of forces in directions orthogonal to Σ.

For application to problems other than those in which *all* the collective coordinates are cyclic (ignorable), we deduce in Sec. III, a set of first order partial differential equations characterizing the surface Σ. These equations imply that Σ, if it exists, is a generalized valley (a concept discussed in the Appendix). However, in general, a prescribed Hamiltonian may not admit an exactly decoupled motion of the type specified. This manifests itself in that the deduced partial differential equations are not integrable. Even in this case, which is relevant for most physics problems, we propose a modified procedure: We replace the original equations by a modified set which usually has a solution consisting of the points of a surface Σ and a plane associated with each point. The integrability condition, which is also the condition for a fully decoupled motion, is that these planes be the tangent planes to the surface. By introducing a measure of deviation from tangency, we arrive at a concept of approximate decoupling, useful for physics applications. The collective Hamiltonian can be constructed from the exact solution of the modified set of equations. Further discussion for the case of additional constants of the motion is carried out.

In the Appendix, some geometrical properties are described. First we discuss briefly the concept of generalized valley. We then prove that integrability of the equations requires that Σ be a geodesic surface ("minimum" area for $K\geq 2$, minimum length for $K=1$) in the geometry of the original N dimensional space.

II. DECOUPLED CLASSICAL MOTIONS

A. Preliminaries

We study a classical system described by N canonical pairs $(\xi^\alpha,\pi_\alpha)=(\underline{\xi},\underline{\pi})$, $\alpha=1\ldots$N and a Hamiltonian quadratic in the π_α,

$$H(\underline{\xi},\underline{\pi})=\tfrac{1}{2}\pi_\alpha B^{\alpha\beta}(\underline{\xi})\pi_\beta+V(\underline{\xi}) , \tag{2.1}$$

which is characterized by the potential energy surface $V(\underline{\xi})$ and the mass matrix $B^{\alpha\beta}(\underline{\xi})$. We subject the system described by (2.1) to a point canonical transformation (in order to retain the quadratic structure in the momentum variables)

$$\xi^\alpha=g^\alpha(\underline{q}) , \tag{2.2a}$$

$$p_\mu=g^\alpha_{,\mu}\pi_\alpha \tag{2.2b}$$

with inverse

$$q^\mu=f^\mu(\underline{\xi}) , \tag{2.3a}$$

$$\pi_\alpha=f^\mu_{,\alpha}p_\mu . \tag{2.3b}$$

Here the notation of comma followed by index will be used for differentiation. Thus

$$g^\alpha_{,\mu}=(\partial g^\alpha/\partial q^\mu),\quad f^\mu_{,\alpha}=(\partial f^\mu/\partial \xi^\alpha) . \tag{2.4}$$

Since the $(\underline{\xi},\underline{\pi})$ and the $(\underline{q},\underline{p})$ are the only sets of canonical coordinate which will appear in the theoretical development, they can be distinguished by reserving the indices $\alpha,\beta,\ldots,$ for the $(\underline{\xi},\underline{\pi})$ and $\mu,\nu,\ldots,$ for the $(\underline{q},\underline{p})$ even though both sets of indices run over the same values $1,\ldots,N$. In addition, quantities in the $(\underline{q},\underline{p})$ coordinate system will be distinguished by a bar.

Under the restriction to time-independent transformations, (2.2), the Hamiltonian becomes

$$\bar{H}(\underline{q},\underline{p})=H[\underline{\xi}(\underline{q}),\underline{\pi}(\underline{q},\underline{p})]$$
$$=\tfrac{1}{2}p_\mu \bar{B}^{\mu\nu}p_\nu+\bar{V}(\underline{q})\ , \quad (2.5)$$

where the metric tensor

$$\bar{B}^{\mu\nu}=f^{\mu}_{,\alpha}f^{\nu}_{,\beta}B^{\alpha\beta} \quad (2.6)$$

transforms like a contravariant tensor of second rank. We shall also be interested in the covariant form of (2.6), namely

$$\bar{B}_{\mu\nu}=g^{\alpha}_{,\mu}g^{\beta}_{,\nu}B_{\alpha\beta}\ , \quad (2.7)$$

where $B_{\alpha\beta}$ is both the covariant form of $B^{\alpha\beta}$ and the matrix inverse to it.

The point character of the transformation (2.2) and (2.3) is expressed by the chain rule relations

$$\delta^{\mu}_{\nu}=f^{\mu}_{,\alpha}g^{\alpha}_{,\nu}\ , \quad (2.8a)$$

$$\delta^{\alpha}_{\beta}=g^{\alpha}_{,\mu}f^{\mu}_{,\beta}\ . \quad (2.8b)$$

From (2.8b) and (2.6) we have

$$g^{\alpha}_{,\mu}\bar{B}^{\mu\nu}=B^{\alpha\beta}f^{\nu}_{,\beta}\ . \quad (2.9)$$

For reasons to be discussed following Eq. (2.13) below, let us consider the equations of motion expressed in the two equivalent ways,

$$\dot{\xi}^{\alpha}=(\partial H/\partial\pi_\alpha)=\{\xi^\alpha,\bar{H}\}\ , \quad (2.10a)$$

$$\dot{\pi}_\alpha=-(\partial H/\partial\xi^\alpha)=\{\pi_\alpha,\bar{H}\}\ , \quad (2.10b)$$

where the curly brackets are read as a Poisson bracket with respect to the set $(\underline{q},\underline{p})$. Thus, in writing (2.10) we recognize the ξ^α,π_α both as canonical variables and as dynamical functions of the q^μ,p_μ. If after carrying out differentiations, we substitute into (2.10) the transformation equations (2.2a) and (2.3b), the second equality in each of (2.10a) and (2.10b) become, respectively,

$$g^{\alpha}_{,\mu}\bar{B}^{\mu\nu}p_\nu=B^{\alpha\beta}f^{\nu}_{,\beta}p_\nu \quad (2.11)$$

[which is instantly recognized as an identity in view of (2.9)] and

$$V_{,\alpha}+\tfrac{1}{2}p_\mu p_\nu f^{\mu}_{,\beta}f^{\nu}_{,\gamma}B^{\beta\gamma}_{,\alpha}$$
$$=f^{\mu}_{,\alpha}(\bar{V}_{,\mu}+\tfrac{1}{2}p_\nu p_\lambda \bar{B}^{\nu\lambda}_{,\mu})-p_\nu p_\lambda f^{\lambda}_{,\alpha\beta}g^{\beta}_{,\mu}\bar{B}^{\mu\nu}\ . \quad (2.12)$$

This equation must also be an indentity, since point transformations are automatically canonical when the transformed Hamiltonian is defined by (2.5) and thus no new conditions should emerge. The momentum independent terms evidently cancel, using the chain rule, whereas if we substitute (2.11) into the last term of (2.12) the momentum dependent terms can be put into the form

$$(f^{\mu}_{,\beta}f^{\nu}_{,\gamma}B^{\beta\gamma})_{,\alpha}=\bar{B}^{\mu\nu}_{,\lambda}f^{\lambda}_{,\alpha} \quad (2.13)$$

which is just a derivative of (2.6).

The reason for carrying out the exercise just completed is that as soon as we place special additional constraints on the point transformation, as we shall below, and enforce these constraints on (2.11) and (2.12), we shall find that these equations, rather than remaining identities, become conditions for the determination of the special point transformations satisfying these additional constraints.

B. Description of decoupled classical motion

We can now reveal the origin of our interest in studying the point transformation (2.2), (2.3). We divide the new coordinates into two sets, (q^i,p_i), $i=1,\ldots,K$ and (q^a,p_a), $a=K+1,\ldots,N$, and ask: Does the system admit a point transformation and an integer K with the following property: Given $q^a=p_a=0$ at $t=0$, are there motions in which these coordinates and momenta remain zero for all times? Now the conditions $q^a=0$ reduce (2.2a) to the equations for a K-dimensional surface Σ, in an N-dimensional space. Thus we may rephrase the conditions: Given that ξ^α is initially on Σ and $\dot{\xi}^\alpha=g^{\alpha}_{,\mu}\dot{q}^{\mu}$ is initially on $T\Sigma$, the tangent plane to Σ at the given point, we wish to characterize such classical motions for which the system point remains forever on Σ. This is the definition of K-dimensional decoupled classical motion.

To obtain conditions for the determination of Σ, we note that the requirements that $q^a(t)=p_a(t)=0$ imply that $\bar{H}(q^i,q^a=0,p_i,p_a=0)\equiv\bar{H}(q^i,p_i)$ is the Hamiltonian for motion on Σ. This observation may now be applied to Hamilton's equations (2.10) restricted to the surface Σ, namely,

$$(\partial H/\partial\pi_\alpha)\,|_{\Sigma}=\{\xi^\alpha,\bar{H}(q^i,p_i)\}\ , \quad (2.14a)$$

$$-(\partial H/\partial\pi^\alpha)\,|_{\Sigma}=\{\pi_\alpha,\bar{H}(q^i,p_i)\}\ , \quad (2.14b)$$

where the Poisson brackets involve differentiation only with respect to the set (q^i,p_i). Following the same reasoning used on conjunction with (2.10), but remembering that (2.2) and (2.3) are restricted to the surface Σ, we obtain from (2.14) the conditions

$$B^{\alpha\beta}f^{j}_{,\beta}=g^{\alpha}_{i,}\bar{B}^{ij}\ , \quad (2.15)$$

$$V_{,\alpha}+\tfrac{1}{2}p_ip_jf^{i}_{,\beta}f^{j}_{,\gamma}B^{\beta\gamma}_{,\alpha}$$
$$=f^{k}_{,\alpha}(\bar{V}_{,k}+\tfrac{1}{2}p_ip_j\bar{B}^{ij}_{,k})-p_ip_jf^{i}_{,\alpha\beta}g^{\beta}_{,k}\bar{B}^{kj}\ . \quad (2.16)$$

If we substitute (2.15) into the last term of (2.16), the latter equation may be rewritten as

$$(V+\tfrac{1}{2}p_ip_jB^{ij})_{,\alpha}=f^{k}_{,\alpha}(\bar{V}_{,k}+\tfrac{1}{2}p_ip_j\bar{B}^{ij}_{,k})\ . \quad (2.17)$$

Further information is to be obtained by comparing (2.15) and (2.17) with (2.11) and (2.12) when the latter are specialized to a surface Σ. Because in the evaluation of (2.11) [or (2.9)] and (2.12) no *a priori* restrictions have been placed on $\bar{H}-\Sigma$ is here any K-dimensional surface—we expect and find additional terms not present in (2.15) and (2.17). If Σ is a decoupled surface these additional contributions must be required to vanish. For example, comparison of (2.9) with $\nu=j$ with (2.15) then implies that

$$g^{\alpha}_{,a}\bar{B}^{aj}=0 \ , \tag{2.18}$$

or with the help of (2.8a),

$$\bar{B}^{ai}=\bar{B}^{ia}=0 \ . \tag{2.19}$$

Correspondingly, with the help of (2.15) and (2.19), (2.12) may be rewritten

$$(V+\tfrac{1}{2}p_ip_jB^{ij})_{,\alpha}=f^{k}_{,\alpha}(\bar{V}_{,k}+\tfrac{1}{2}p_ip_j\bar{B}^{ij}_{,k}) + f^{a}_{,\alpha}(\bar{V}_{,a}+\tfrac{1}{2}p_ip_j\bar{B}^{ij}_{,a}) \ . \tag{2.20}$$

Comparison with (2.17) [and the application of (2.8a)] yields the conditions

$$\bar{V}_{,a}+\tfrac{1}{2}p_ip_j\bar{B}^{ij}_{,a}=0 \ . \tag{2.21}$$

To understand what has been accomplished, we make a distinction between two cases. In the first case, which is the only one we have studied previously[29] we assume that none of the coordinates q^i is cyclic, nor can they be made so by a suitable choice of coordinates on Σ, i.e., there are no conserved quantities p_i. Under these circumstances, because p_i are variable independently for fixed coordinates, both (2.17) and (2.21) provide two sets of equations; the coefficients of unity and the coefficients of p_ip_j may be equated separately. In this case we can present our results as two lists of conditions, which are equivalent:

$$\bar{B}^{ia}=\bar{B}^{ai}=0 \leftrightarrow B^{\alpha\beta}f^{i}_{,\beta}=\bar{B}^{ij}g^{\alpha}_{,j} \ , \tag{2.22}$$

$$\bar{V}_{,a}=0 \leftrightarrow V_{,\alpha}=f^{i}_{,\alpha}\bar{V}_{i,} \ , \tag{2.23}$$

$$\bar{B}^{ij}_{,a}=0 \leftrightarrow \bar{B}^{ij}_{,\alpha}=\bar{B}^{ij}_{,k}f^{k}_{,\alpha} \ . \tag{2.24}$$

We can use the corresponding member of either set, as convenient.

The physical meaning of these conditions is seen most clearly from the list on the left-hand side. Provided the metric tensor has been chosen block diagonal as required by (2.22), (2.23) signifies the absence of "real" forces, orthogonal to Σ, whereas (2.24) specifies the absence of centrifugal forces perpendicular to Σ. Thus "physical" and geometrical forces tending to force the system off the decoupled surface must be absent, independently of one another, for decoupled motion to occur when none of the collective momenta is a constant of the motion. (This will contrast below with the situation when there are additional constants of the motion.)

In the next section we shall explore mathematically how these conditions determine the surface Σ. Before doing so, we must recognize how they are altered when there are symmetries of the original Hamiltonian. As we shall see, one encounters here a situation in which the system point is confined to Σ by a partial (or in an extreme case total) balance between applied and centrifugal forces orthogonal to the collective surface, rather than the absence of both components. In order to elucidate this case, let us suppose that, if necessary, a preliminary (point) transformation has been carried out so that all the conserved quantities appear explicitly among the π_α, and therefore the corresponding ξ^α are cyclic (ignorable). This is particularly convenient whenever we look for solutions which include one or more of these cyclic variables in the description of points on the surface. For such values of α, the corresponding Eq. (2.17) becomes a *trivial identity*: Since ξ^α is already a collective coordinate and cyclic, $\xi^\alpha \rightarrow q^i$, both sides of this equation are identically zero under these circumstances because V, $\bar{V}$, $B^{\alpha\beta}$, and $\bar{B}^{\mu\nu}$ are independent of $\xi^\alpha=q^i$.

The implication is that in such a case we are missing some equations necessary to determine Σ. To see that that is so, let us consider an extreme situation where all the q^i are cyclic. Then there is no information at all in (2.17). How shall we determine the surface Σ? The solution lies in Eq. (2.21). The assumption that we have identified the cyclic q^i implies normally that we also can construct explicitly a set of q^a. The equations (2.21) are (N-K) equations, which for *constant* p_i, determine ($N-K$) vales q^a. (By redefinition they may be taken to be $q^a=0$.) Since p_a has already been set to zero, we see that in this extreme case, (2.21) by itself determines the surface Σ, $q^a=p_a=0$.

To illustrate with a familiar case, consider the Hamiltonian

$$H=\tfrac{1}{2}(p_x^2+p_y^2)+V[(x^2+y^2)^{1/2}] \ . \tag{2.25}$$

This Hamiltonian admits two classes of decoupled motion, circular motion with constant speed and radial motion. We are intested here in the circular motion, where with $p=l=$angular momentum and $q^a=\rho=(x^2+y^2)^{1/2}$, Eq. (2.21) is just the well-known condition for the radius and this motion.

The general case, where some coordinates of Σ are cyclic and others not, uses a mixture of (2.21) and (2.23), (2.24) which is best elucidated in conjunction with the geometrical theory to be developed in Sec. III. We thus postpone further discussion.

C. Alternative equivalent formulations

We first exhibit a simple alternative derivation of the left-hand list of Eqs. (2.22)–(2.24). Suppose we expand $\bar{H}(q,p)$ about its value on some K dimensional surface Σ. We obtain from (2.5)

$$\begin{aligned}\bar{H} &\cong \bar{H}\,|_{\Sigma}+\left.\frac{\partial\bar{H}}{\partial q^a}\right|_{\Sigma}q^a+\left.\frac{\partial\bar{H}}{\partial p_a}\right|_{\Sigma}p_a+\text{quadratic terms}\\ &=\bar{H}\,|_{\Sigma}+(\bar{V}_{,a}+\tfrac{1}{2}p_ip_j\bar{B}^{ij}_{,a})q^a+\bar{B}^{ia}p_ip_a+\cdots \ .\end{aligned} \tag{2.26}$$

The requirement that the coefficients of q^a and p_a vanish are precisely Eqs. (2.21) and (2.22) and thus shed another light on the conditions for existence of decoupled classical motion. This approach also calls to one's attention the importance of the quadratic terms which alone will determine whether and to what extent a decoupled motion is actually stable.

A second observation is that Eqs. (2.14) may be viewed as variational approximations to the full Hamilton's equation. This point was originally made at the quantum level.[26] The classical limit of that remark will now be derived independently from Hamilton's principle in the form

$$\delta I=\delta\int_{t_0}^{t_1}(\pi_\alpha\dot{\xi}^\alpha-H)dt=0\ . \tag{2.27}$$

We look for the best solution when $\xi^\alpha=\xi^\alpha(q^i)$ is confined to a surface Σ. The equations

$$\dot{\xi}^\alpha=\{\xi^\alpha,\bar{H}\}\ , \tag{2.28a}$$

$$\dot{\pi}_\alpha=\{\pi_\alpha,\bar{H}\} \tag{2.28b}$$

define $\bar{H}$ as the generator of time translations on Σ. Carrying out the variation of (2.27) in the standard way and substituting (2.28), we find

$$\delta I=\int_{t_0}^{t_1}\{\delta\pi_\alpha[\{\xi^\alpha,\bar{H}\}-(\partial H/\partial\pi_\alpha)] +\delta\xi^\alpha[-\{\pi^\alpha,\bar{H}\}-(\partial H/\partial\xi^\alpha)]\}\ , \tag{2.29}$$

which yields (2.14) and its consequences.

III. CONSTRUCTION OF THE COLLECTIVE HYPERSURFACE

A. Characterization of the tangent planes to the decoupled (collective) surface

It follows from the definition of the surface Σ that the quantities $g^\alpha_{,j}$ constitute for fixed j the components of a tangent vector to this surface. There are K such vectors, $j=1\ldots K$. When Eqs. (2.22) are satisfied (consider the right hand set), it is equivalent that the quantities $f^i_{,\beta}$ also constitute a set of K basis vectors for the tangent plane. Then Eq. (2.23) states that ∇V (gradient of V) lies in the tangent plane.

We shall now show that provided Eqs. (2.22)–(2.24) are satisfied ∇V is the first of an indefinite number of tangent vectors that can be formed from V and from $B^{\alpha\beta}$, the "ingredients" of the given Hamiltonian. We define a sequence of point functions

$$^{(1)}X=V\ , \tag{3.1}$$

$$^{(2)}X\equiv U\equiv\tfrac{1}{2}V_{,\alpha}B^{\alpha\beta}B_{,\beta}\ , \tag{3.2}$$

$$^{(3)}X\equiv W\equiv\tfrac{1}{2}U_{,\alpha}B^{\alpha\beta}U_{,\beta}\ , \tag{3.3}$$

$$^{(\sigma)}X\equiv\tfrac{1}{2}{}^{(\sigma-1)}X_{,\alpha}B^{\alpha\beta(\sigma-1)}X_{,\beta}\ . \tag{3.4}$$

For application below, it is convenient to express these quantities in terms of the new coordinates,

$$^{(\sigma)}X\equiv{}^{(\sigma)}\bar{X}=\tfrac{1}{2}{}^{(\sigma-1)}\bar{X}_{,\mu}\bar{B}^{\mu\nu(\sigma-1)}\bar{X}_{,\nu}\ . \tag{3.5}$$

Theorem. Let Eqs. (2.22)–(2.24) be satisfied and assume provisionally that on Σ, for arbitrary σ,

$$^{(\sigma-1)}\bar{X}_{,a}=0\ . \tag{3.6}$$

Then we shall prove that $^{(\sigma)}\bar{X}_{,a}=0$. To see this we calculate from (3.5)

$$\begin{aligned}^{(\sigma)}\bar{X}_{,a}&={}^{(\sigma-1)}\bar{X}_{,\mu a}{}^{(\sigma-1)}\bar{X}_{,\nu}\bar{B}^{\mu\nu}+\tfrac{1}{2}{}^{(\sigma-1)}\bar{X}_{,\mu}{}^{(\sigma-1)}\bar{X}_{,\nu}\bar{B}^{\mu\nu}_{,a}\\&={}^{(\sigma-1)}\bar{X}_{,ai}{}^{(\sigma-1)}\bar{X}_{,j}\bar{B}^{ij}\\&\quad+\tfrac{1}{2}{}^{(\sigma-1)}\bar{X}_{,i}{}^{(\sigma-1)}\bar{X}_{,j}\bar{B}^{ij}_{,a}=0\ .\end{aligned} \tag{3.7}$$

In the first rewriting of (3.7), we have utilized (3.6) and (2.22) and in reaching the value zero, we have again used (3.6) and $\Sigma({}^{(\sigma-1)}\bar{X}_{,a}=0\rightarrow{}^{(\sigma-1)}\bar{X}_{,ai}=0)$ and (2.24). Notice next that for $\sigma=2$, we do not need (3.6) as a separate assumption, since (2.23) provides the necessary condition. Thus using induction, Eqs. (2.22)–(2.24) are sufficient to establish the results

$$^{(\sigma)}\bar{X}_{,a}=0\leftrightarrow{}^{(\sigma)}X_{,\alpha}=f^i_{,\alpha}{}^{(\sigma)}\bar{X}_{,i}\ , \tag{3.8}$$

i.e., $\nabla^{(\sigma)}X$ lies in the tangent plane for any σ. [The set of tangent vectors is even larger, see (3.22) below, but the set $\nabla^{(\sigma)}X$ suffices for present purposes.]

This theorem establishes the foundation for an explicit determination of the collective surface Σ. We have already remarked that the K tangent vectors $f^i_{,\alpha}, i=1,\ldots,K$ provide a basis for the tangent plane $T\Sigma$. The $(K+1)$ vectors $\nabla^{(\sigma)}X,=1,\ldots,K+1$ which lies in $T\Sigma$ must therefore be linearly dependent, i.e., we can write

$$V_{,\alpha}-\sum_{\sigma=2}^{K+1}\Omega_{(\sigma-1)}{}^{(\sigma)}X_{,\alpha}+0\ . \tag{3.9}$$

As we shall illustrate shortly, the elimination of the "Lagrange multipliers" $\Omega_{(\sigma)}$ (see the Appendix) provides a set of determinantal conditions which are explicit equations for the surface $\xi^\alpha=g^\alpha(q^i)$ and not differential characterizations of them, as in Eq. (3.8). Equation (3.9) is the equation which we solve in practice (see below and the accompanying paper), but there remain a number of theoretical questions to be answered.

Before studying these questions, we first illustrate the application of (3.9) to the case $N=3,K=2$, utilizing the notation $V,U,W,\ldots$ defined in (3.1)–(3.3). The elimination of $\Omega_{(1)}$ and $\Omega_{(2)}$ from (3.9) yields the determinantal condition

$$\begin{vmatrix}V_{,1}&V_{,2}&V_{,3}\\U_{,1}&U_{,2}&U_{,3}\\W_{,1}&W_{,2}&W_{,3}\end{vmatrix}=0\ , \tag{3.10}$$

which is the familiar condition that ∇V, ∇U, and ∇W lie in a plane. To solve this equation for the surface

$$\xi^\alpha=g^\alpha(q^1,q^2),\quad\alpha=1,2,3\ , \tag{3.11}$$

it is convenient to utilize the parametrization $\xi^i=q^i$, $i=1,2$, and

$$\xi^3=\phi(\xi^1,\xi^2)\ . \tag{3.12}$$

In an accompanying paper, we shall present a detailed study of just such an example.

B. Measure of decoupling: Collective Hamiltonian

As stated above, we propose in practice to solve (3.9), or the equivalent equations obtained by eliminating the $\Omega_{(\sigma)}$, in order to find candidates for the collective surface Σ, as expressed by the equations $\xi^\alpha = g^\alpha(q^i)$. Tangent vectors $g^\alpha_{,j}$ may then be computed directly. But now we must recall that (3.9) plays the role of consistency conditions for the solution of (3.8). A nontrivial solution of (3.9) will guarantee a nontrivial solution of (3.8) for the quantities $f^i_{,\alpha}$, and herein lies the crux of the matter.

To see the point involved most clearly, let us rewrite (3.8) by means of (2.22). With the definitions

$$^{(\sigma)}X^{,\alpha} = B^{\alpha\beta(\sigma)}X_{,\beta} \ , \tag{3.13}$$

$$^{(\sigma)}\bar{X}^{,i} = \bar{B}^{ij(\sigma)}\bar{X}_{,j} \ , \tag{3.14}$$

we have as the contravariant form of (3.8),

$$^{(\sigma)}X^{,\alpha} = {}^{(\sigma)}\bar{X}^{,i} g^\alpha_{,i} \ . \tag{3.15}$$

To solve these equations for $g^\alpha_{,i}$, we must eliminate the unknowns $^{(\sigma)}\bar{X}^{,i}$. This can be done, for example, with the aid of a general covariance property of the theory: Given any choice of the variables q^i which characterize the surface Σ, the form of the theory, i.e., of Eqs. (3.15), must be invariant under a point canonical transformation *on the surface* Σ. This is easy to show explicitly[26] and is implied correctly by the notation in (3.15) which indicates that we have a scalar product with respect to the indices i. This means that K of the N equations defining the surface may be chosen arbitrarily, for example, the functions $(i = 1, \ldots, K)$

$$\xi^i = g^i(\underline{q}) \ . \tag{3.16}$$

For the clarity of the present discussion, the simplest choice for (3.16) is [a generalization of (3.11) and (3.12)]

$$\xi^i = q^i \ ,$$

$$\xi^a = g^a(\xi^1 \ldots \xi^K), \quad a = K+1, \ldots \ . \tag{3.17}$$

Equations (3.16) and (3.17) now imply for (3.15) that

$$^{(\sigma)}X^{,i} = {}^{(\sigma)}\bar{X}^{,i} \ , \tag{3.18}$$

and

$$^{(\sigma)}X^{,a} = {}^{(\sigma)}X^{,i} g^a_{,i} \ . \tag{3.19}$$

Equation (3.9) remains the condition for the consistency of (3.19). Inserting the solution of (3.9) into (3.19), a set of quantities, nominally identified as $g^a_{,i}$ can be computed (the $g^j_{,i}$ have been chosen). Since we already have an integral surface $\xi^\alpha = g^\alpha(q)$ from the solution of (3.9), the tangent vectors can also be computed independently from this source. We see that the procedure we have described provides two ways of computing $T\Sigma$ at each point of the surface Σ which satisfies (3.9). (That which is computed directly is naturally $T\Sigma$.) These two computations may or may not agree.

Thus for full consistency of the theory, we have the requirement that Eqs. (3.19) determine a surface and at the same time the tangent plane to it at every point. But we must face physical reality: In realistic applications, truly decoupled motions will be few and far between. Does this imply that we have constructed a useless edifice? For the remainder of this section we discuss a basis for adopting a more optimistic view.

Let us first change possible inconsistency back to consistency by replacing (3.19) by the equations

$$^{(\sigma)}X^{,a} = {}^{(\sigma)}X^{,i}\gamma^a_i \ . \tag{3.20}$$

We view the γ^α_i for fixed i and $\gamma^j_i = \delta^j_i$ as defining for any solution of (3.9) a set of basis vectors γ_i which determine a plane $P\Sigma$ associated with each point of Σ. In general $P\Sigma \neq T\Sigma$. It seems reasonable, however, to introduce a local measure of error which may indicate the extent to which the solution of (3.20) yields an approximately decoupled classical motion. We suggest the following scale invariant measure: Let

$$\delta^\alpha_i = g^\alpha_{,i} - \gamma^\alpha_i \ . \tag{3.21}$$

Then

$$D(\underline{q}) \equiv \frac{\delta^\alpha_i B_{\alpha\beta}\bar{B}^{ij}\delta^\beta_j}{g^\alpha_{,i}B_{\alpha\beta}\bar{B}^{ij}g^\beta_{,j}} \tag{3.22}$$

is a reasonable invariant measure of decoupling (though not a unique one). Further discussion and evaluation of validity criteria are given in the accompanying paper, but it is appropriate to explain here the function of (3.22).

Toward this end it is well to remind ourselves that what we are after, ultimately, is the collective Hamiltonian, i.e., the Hamiltonian which governs the motion on Σ. According to the method proposed, we have

$$\bar{V}(q^1, \ldots, q^K) \equiv V[g^1(\underline{q}), \ldots, g^N(\underline{q})] \ , \tag{3.23}$$

unambiguously. For the metric tensor, experience suggests that we calculate it from the elements of $T\Sigma$, using the formula

$$\bar{B}_{ij} = g^\alpha_{,i}B_{\alpha\beta}g^\beta_{,j} \ , \tag{3.24}$$

which can be derived from (2.8a) and (2.22). Since we could have used the quantities γ^α_i in (3.24), it is clear that the criterion (3.22) measured the extent to which (3.24) is essentially unique, and thus provides further support for the introduction of Eq. (3.22) as a criterion of validity.

C. An inverse theorem

We have described a method of calculating the collective surface Σ by solving (3.8) [or in practice (3.20)]. For practical purposes, we have thus replaced (2.22)–(2.24) by (2.22) and the set (3.8). This leads us naturally to ask: When (3.8) has fully consistent solutions does this prove that (2.23) and (2.24) are satisfied, i.e., does this establish a decoupled motion? We shall prove that this is true except in the event that the original Hamiltonian has additional constants of the motion besides the energy. In the latter case this "inverse theorem" fails, a welcome result in the light of the fact that (2.23) and (2.24) are no longer fully correct! We have already implied that in that event the consequences of (2.21) are modified because *some* of the p_i are fixed rather than arbitrary. Depending on the detailed Hamiltonian, for some values of the noncollective indices a, we still have (2.23) and (2.24), whereas for others (2.21) must be considered as a whole. For these latter values we have a balance of applied and centrifugal forces, as illustrated in the example based on Eq. (2.25).

Let us recall that the first of Eqs. (3.8) coincides with (2.23). Thus, we wish to prove that the remaining members of (3.8) imply that $\bar{B}^{ij}_{,a}=0$. Furthermore we expect this proof to break down in part or in whole when there are additional constants of the motion. We turn then to the details of the demonstration.

We consider the computation of ${}^{(\sigma)}X_{,\alpha}$ from (3.5). This computation parallels that given in (3.7). If we do not insist on (2.23) and (2.24), but wish to derive (3.8) (right-hand form), we must require the additional terms that arise in this calculation, which appear as the coefficients of $f^{a}_{,\alpha}$, to vanish, namely

$$ {}^{(\sigma+1)}\bar{X}_{,a}={}^{(\sigma)}\bar{X}_{,\mu a}\bar{B}^{\mu\nu(\sigma)}\bar{X}_{,\nu} + \tfrac{1}{2}{}^{(\sigma)}\bar{X}_{,\mu}\bar{B}^{\mu\nu(\sigma)}_{,a}\bar{X}_{,\nu}=0 \;. \quad (3.25)$$

Equation (3.25) applies to all but the first of Eqs. (3.8), which, as remarked above, coincides with (2.23). It is thus left to prove that the set (3.25) implies (2.24). Now the first term of (3.25) equals ${}^{(\sigma)}\bar{X}_{,ba}\bar{B}^{bi(\sigma)}\bar{X}_{,i}=0$, since ${}^{(\sigma)}\bar{X}_{,a}=0$ and $\bar{B}^{ai}=0$. Therefore Eqs. (3.25) reduce to the equations

$$\bar{B}^{ij}_{,a}{}^{(\sigma)}\bar{X}_{,i}{}^{(\sigma)}\bar{X}_{,j}=0 \;. \quad (3.26)$$

Before attempting to reach any conclusions, we must draw attention to the fact that the list $\nabla^{(\sigma)}X$ of tangent vectors is not sufficiently complete for present purposes. We define the point functions ($\sigma\neq\tau$)

$${}^{(\sigma\tau)}Y={}^{(\sigma\tau)}\bar{Y}=\bar{B}^{\mu\nu(\sigma)}\bar{X}_{,\mu}{}^{(\tau)}\bar{X}_{,\nu} \;, \quad (3.27)$$

which includes the previous set ${}^{(\sigma)}X$. It is then easily shown, as in (3.7), that $\nabla^{(\sigma\tau)}Y$ is a tangent vector. Furthermore following the arguments leading to (3.25) and (3.26), we can obtain a generalized form of the latter:

$$\bar{B}^{ij}_{,a}{}^{(\sigma)}\bar{X}_{,i}{}^{(\tau)}\bar{X}_{,j}=0 \;. \quad (3.28)$$

To understand the content of (3.28), we consider first the simplest cases. For one-dimensional decoupled motion, it suffices to consider $\sigma=\tau=1$, namely

$$\bar{B}^{11}_{,a}(\bar{V}_{,1})^2=0 \;. \quad (3.29)$$

If $\bar{V}_{,1}\neq 0$, we obtain the desired result, $\bar{B}^{11}_{a}=0$. However, if $\bar{V}_{,1}=0$, then q^1 is a cyclic variable. In this case ∇V is orthogonal to the collective path and therefore cannot determine it. The required modification of the previous theory will be described in Sec. III D.

For two dimensional decoupled motion, we consider the equations for $\sigma,\tau=1,2$. We get three sets of conditions:

$$\bar{B}^{ij}_{,a}\bar{V}_{,i}\bar{V}_{,j}=0, \quad i,j=1,2 \quad (3.30a)$$

$$\bar{B}^{ij}_{,a}\bar{V}_{,i}\bar{U}_{,j}=0 \;, \quad (3.30b)$$

$$\bar{B}^{ij}_{,a}\bar{U}_{,i}\bar{V}_{,j}=0 \;. \quad (3.30c)$$

For each value of a, these are three linear homogeneous equations for the three variables $\bar{B}^{ij}_{,a}$, which will have the trivial solution provided the determinant

$$\Delta_2=\begin{vmatrix}\bar{V}_{,1} & \bar{V}_{,2}\\ \bar{U}_{,1} & \bar{U}_{,2}\end{vmatrix}\neq 0 \;, \quad (3.31)$$

the actual determinant of the coefficients in (3.30) being the third power of Δ_2. If $\Delta_2=0$, the previous theory is incomplete and we have one of two cases. Either ∇V is parallel to ∇U and we have one constant of the motion or $\bar{V}_{,1}$ and $\bar{V}_{,2}$ both vanish and we have two constants of the motion.

The examples we have given generalize. For a K-dimensional decoupled motion, provided there are no additional conserved quantities on Σ, the theory described by (3.8) and (2.22) is complete and equivalent to the conditions (2.22)–(2.24). *Otherwise we must re-examine the derivation of (2.23) and (2.24).* We describe very sufficiently how this is to be done.

D. Modification of the theory for conserved quantities

The derivation of (2.23) and (2.24) depended on being able to equate to zero separately in (2.21) the coefficients of unity and of p_ip_j. When the p_i are not constants of the motion, they may, be suitably choice of initial conditions take on a range of values at a given space point, thus justifying the conclusions drawn. When a subset of the p_i takes constant values for the entire surface, this reasoning must be modified as follows: Let there be $K_1\leq K$ conserved quantities on Σ, with $p_i=c_i$, $i=1,\ldots,K_1$. As a generalization from simple examples, it is assumed that a preliminary point transformation has been carried out introducing the $q^i\equiv\theta^i$, $i=1,\ldots,K_1$ as cyclic variables and K_1 "associated" noncollective variables ρ^a, $a=K+1,\ldots,K+K_1$, and that the $\bar{B}^{ij}$ are known function of ρ^a, again only for $i,j=1,\ldots,K_1$. Then we can choose a subset of the Eqs. (2.21) in the form

$$(\partial\bar{V}/\partial\rho^a)+\tfrac{1}{2}c_ic_j(\partial\bar{B}^{ij}/\partial\rho^a)=0 \;. \quad (3.32)$$

These determine the ρ^a as functions of the q^i, $i=K_1+1,\ldots,K$ for fixed c_i. The machinery leading to (2.22)–(2.24) and then subsequently to (3.8) can be applied to finding a "reduced" surface Σ_R of dimension $(K-K_1)$ out of $N-2K_1$ variables. More explicitly we can write

$$H=\tfrac{1}{2}\sum_{i,j=1}^{K_1}\bar{B}^{ij}p_ip_j+\tfrac{1}{2}\sum_{a,b=K+1}^{K+K_1}\bar{B}^{ab}p_ap_b+H_R \;, \quad (3.33)$$

$$H_R=\tfrac{1}{2}\sum_{\alpha,\beta=K_1+1}^{N-2K_1}\pi_\alpha\pi_\beta B^{\alpha\beta}(\underline{\xi})+V(\rho^a,\xi^\alpha) \;. \quad (3.34)$$

The point is that for the theory starting with Eq. (2.14), we substitute H_R for H, the ρ^a being held fixed at values ultimately determined by (3.32).

The method developed in this section will be referred to henceforth as the generalized valley approximation (GVA). The reason for this name is discussed in the appendix, where it is tied to the geometrical significance of (3.9).

IV. APPLICATION TO A MONOPOLE-DIPOLE MODEL

In a following paper we present some numerical studies in which we solve the GVA equations and study the solutions. Here we will consider a simple analytic example. For the reader who has no interest in the algebraic details, we summarize what is demonstrated below. We study an example based on the Hamiltonian (4.1) as modified by (4.11), which admits exactly decoupled classical motions in a plane described by Eq. (4.24). The equations of the generalized valley, either (2.22)–(2.24) or (3.19) are thereby satisfied exactly. In other words, these equations are integrable in this case and the decoupled surface Σ can be constructed.

By way of introduction, we study the Hamiltonian

$$H=\sum_{\alpha=1}^{N}\tfrac{1}{2}(\pi_\alpha^2+\omega_0^2\xi_\alpha^2)+\bar{V}(R)\ , \tag{4.1}$$

where

$$R^2=\sum_\alpha(\xi_\alpha)^2\ . \tag{4.2}$$

It is natural to introduce R as a collective variable. The associated mass is

$$\bar{B}^{\,11}=\frac{\partial R}{\partial\xi_\alpha}\frac{\partial R}{\partial\xi_\alpha}=1\ . \tag{4.3}$$

The tangent vector to the collective path can be calculated from Eq. (2.22),

$$\bar{B}^{\,11}(\partial\xi^\alpha/\partial R)=(\partial R/\partial\xi^\alpha)=(\xi_\alpha/R)\equiv e_\alpha\ , \tag{4.4}$$

or if we consider e_α constant,

$$\xi_\alpha=e_\alpha R\ , \tag{4.5}$$

$$\sum_{\alpha=1}^{N}e_\alpha^2=1\ . \tag{4.6}$$

Of course, (4.5) is simply the point transformation to hyperspherical coordinates, where e_α are direction cosines and we may take $(N-1)$ of them as a set of noncollective coordinates. We have

$$(\partial e_\alpha/\partial\xi_\beta)=(\delta_{\alpha\beta}-e_\alpha e_\beta)/R\ , \tag{4.7}$$

and

$$\bar{B}^{\,1a}=\bar{B}^{\,a1}=0\quad(a\neq1)\ , \tag{4.8}$$

$$\bar{B}^{\,ab}=\bar{B}^{\,ba}=(\delta_{ab}-e_a e_b)/R^2\ . \tag{4.9}$$

Thus the kinetic energy separates

$$\sum_\alpha\tfrac{1}{2}=\pi_\alpha^2=\tfrac{1}{2}P_R^2+\tfrac{1}{2}\sum_{a,b=2}^{N}\bar{B}^{\,ab}P_aP_b\ . \tag{4.10}$$

What we wish to emphasize concerning these well-known formulas is that the conditions for exact decoupling of radial motions are trivially satisfied.

We next turn to our main illustration, which should illuminate all the main points at issue. We have again the form (4.1) with the replacement

$$\bar{V}=\bar{V}(R,D)\ , \tag{4.11}$$

and

$$D=e_\beta\tau_\beta\ , \tag{4.12}$$

$$\tau_\beta\tau_\beta=1\ , \tag{4.13}$$

is a dimensionless dipole coordinate. Here τ_β are the components of an arbitrary unit vector. In general the dependence on D destroys the N-dimensional rotational invariance of (4.1).

Now it is natural to introduce R and D as collective coordinates and to complete the point transformation by an "appropriate" choice of $(N-2)$ noncollective coordinates. First, with $R=q_1$, $D=q_2$, and from

$$(\partial D/\partial\xi_\alpha)=(\tau^\alpha-De^\alpha)/R\ , \tag{4.14}$$

we find

$$\bar{B}^{\,11}=1\ , \tag{4.15}$$

$$\bar{B}^{\,12}=B^{21}=0\ , \tag{4.16}$$

$$\bar{B}^{\,22}=(1-D^2)/R\ . \tag{4.17}$$

We wish to choose $(N-2)$ additional coordinates, q_a, with the property that they give

$$\bar{B}^{\,1a}=\bar{B}^{\,2a}=\bar{B}^{\,a1}=\bar{B}^{\,a2}=0\ . \tag{4.18}$$

Calling these coordinates f_a (4.18) will be satisfied provided

$$e_\alpha(\partial f_a/\partial\xi_\alpha)=0\ , \tag{4.19}$$

$$\tau_\alpha(\partial f_a/\partial\xi_\alpha)=0\ . \tag{4.20}$$

It is an elementary exercise to discover that

$$f_a=(e_a-D\tau_a)/\sqrt{1-D^2}\ . \tag{4.21}$$

There are in fact N of these equations, $\alpha=1,\ldots,N$, which satisfy two constraints

$$f_\alpha\tau_\alpha=0\ , \tag{4.22}$$

$$f_\alpha e_\alpha=\sqrt{1-D^2}\ , \tag{4.23}$$

and as follows from (4.21) the full point transformation has the form (the equation of a plane)

$$\xi_\alpha=e_\alpha(D)R=(f_\alpha\sqrt{1-D^2}+\tau_\alpha D)R\ . \tag{4.24}$$

Equations (4.19) and (4.20) are verified and the elements of the mass matrix in the noncollective space are computed from the formulas

$$(\partial f_\alpha/\partial\xi_\beta)=(\delta_{\alpha\beta}-e_\alpha e_\beta)/R\sqrt{1-D^2}+[(De_\alpha-\tau_\alpha)(\tau_\beta-D_\beta)]/R(1-D^2)^{3/2}\ . \tag{4.25}$$

For what is to follow let us also notice that the tangent vectors are calculated from (4.24) as

$$(\partial\xi_\alpha/\partial R)=e_\alpha \ . \tag{4.26}$$

$$(\partial\xi_\alpha/\partial D)=\frac{R}{1-D^2}(\tau_\alpha-De_\alpha) \ . \tag{4.27}$$

Let us now verify directly that the equations of the generalized valley are exactly satisfied for this example. We have by the chain rule

$$\begin{aligned} V_\alpha &= \frac{\partial V}{\partial R}\frac{\partial R}{\partial \xi_\alpha}+\frac{\partial V}{\partial D}\frac{\partial D}{\partial \xi_\alpha} \\ &= \frac{\partial V}{\partial R}e_\alpha+\frac{1}{R}\frac{\partial V}{\partial D}(\tau_\alpha-De_\alpha) \\ &= \frac{\partial V}{\partial R}\frac{\partial \xi_\alpha}{\partial R}+\frac{(1-D^2)}{R^2}\frac{\partial V}{\partial D}\frac{\partial \xi_\alpha}{\partial D} \ . \end{aligned} \tag{4.28}$$

Then

$$2U=V_\alpha V_\alpha=\left[\frac{\partial V}{\partial R}\right]^2+\frac{1}{R^2}\left[\frac{\partial V}{\partial D}\right]^2(1-D^2)=2U(R,D) \ . \tag{4.29}$$

By differentiating, we find a repetition of (4.28) with $V\to U$. And we repeat once more for W and W_α. Since V_α, U_α, and W_α are at each point, linear combinations of $(\partial\xi_\alpha/\partial R)$ and $(\partial\xi_\alpha/\partial D)$ they do indeed satisfy

$$V_\alpha-\Omega_1(R,D)U_\alpha-\Omega_2(R,D)W_\alpha=0 \ , \tag{4.30}$$

when ξ_α is given by (4.24). The verification (4.28)–(4.30) is, in fact, superfluous since for (4.11), (4.18), and (4.14)–(4.17) we see that Eqs. (2.22)–(2.24) are satisfied!

The calculations carried out above are illustrative of the properties of a broad class of models with decoupled classical motions where we choose to add

$$\bar{V}=\bar{V}(q_1,\ldots,q_K) \quad (K<N) \tag{4.31}$$

to the harmonic oscillator in N dimensions or something equivalently simple, and

$$q_i=q_i(\xi_1,\ldots,\xi_N) \quad (i=1,\ldots,K) \ . \tag{4.32}$$

Furthermore, we can generalize to

$$V=\bar{V}(q_1,\ldots,q_K)+\tilde{V}(q_{K+1},\ldots,q_N) \ , \tag{4.33}$$

provided

$$\frac{\partial q_a}{\partial \xi_\alpha}\frac{\partial q_i}{\partial \xi_\alpha}=0 \ , \tag{4.34}$$

and $\tilde{V}$ satisfies the required stability conditions.

An important point to recognize is that in all the examples of this section, we simply wrote down (by inspection) rather than computed, the equation of the collective surface, which is simply a plane, as required by the considerations developed in the Appendix.

V. SUMMARY AND CONCLUSIONS

Within the context of classical mechanics we have developed a method for approximately decoupling collective degrees of freedom from the Hamiltonian of a many-particle system, the method of the generalized valley. This method has previously been developed only for a single collective coordinate. We have described a theorem necessary to extend the previous considerations to an arbitrary number of collective coordinates, the whole being related to a concept of generalized valley, as described in the Appendix. These results have been illustrated by application to an elementary example.

On the theoretical side, it remains for us to clarify the connection of GVA with the local harmonic approximation. A manuscript dealing with this question is in preparation. For the practical side, we refer, initially, to the following paper.

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APPENDIX: GEOMETRICAL CONSIDERATIONS

1. Generalized valley

A special case of Eq. (3.9), the equation we actually propose to solve for the collective hypersurface, has a well-known geometrical significance, at least for the one-dimensional case. For this case, we have

$$V_{,\alpha}-\Omega_1 U_{,\alpha}=0 \ . \tag{A1}$$

These equations can be associated with the constrained variational principle

$$\delta V-\Omega\delta U=0 \ . \tag{A2}$$

This is one of the definitions for an extremal path on the potential surface. It is more familiar[13] in the equivalent form

$$\delta U-\Lambda\delta V=0 \ , \tag{A3}$$

which invites us to search for stationary values of the magnitude of ∇V along equipotentials of V. This variational principle determines stationary paths including valleys which are the geometrical objects which interest us physically.

We prefer the form (A2) for the following reasons. For $\Omega=0$, this equation reduces to the equation for critical points of V. Thus the critical paths must pass through critical points. When we generalize to higher dimensions, for instance, for two dimensions to the equation

$$\delta V-\Omega_1\delta U-\Omega_2\delta W=0 \tag{A4}$$

[which yields the appropriate form of (3.9)] it is natural to think of this as the definition of a stationary surface of V, including a *generalized valley.* For $\Omega_2=0$, this reduces to the problem of stationary paths, so that we conclude that stationary surfaces must intersect stationary paths. It is clear this argument extends to arbitrary dimensions.

2. Decoupled surface as geodesic

We investigate in a direct manner the consistency of Eqs. (3.8). We illustrate the reasoning with the point function U, which can be written in two ways,

$$U=\tfrac{1}{2}V^{,\alpha}V_{,\alpha}=\tfrac{1}{2}\bar{V}^{,i}\bar{V}_{,i}\ , \tag{A5}$$

where

$$\bar{V}^{,i}=\bar{B}^{ij}\bar{V}_{,j}\ .$$

The first writing is general and the second involves the decoupling conditions. From the latter and the second form of (A5), we can compute

$$U_{,\alpha}=\bar{V}^{;j}_{;i}\bar{V}_{,j}f^{i}_{,\alpha}\ , \tag{A7}$$

where

$$\bar{V}^{;j}_{;i}=\bar{V}^{,j}_{,i}+\gamma^{j}_{ki}\bar{V}^{,k}\ , \tag{A8}$$

and

$$\gamma^{j}_{ki}=\tfrac{1}{2}\bar{B}^{jl}(\bar{B}_{lk,i}+\bar{B}_{li,k}-B_{ki,l}) \tag{A9}$$

is the Christoffel symbol of the second kind on the surface Σ, already defined in Sec. IV.

Next, we calculate $U_{,\alpha}$ using the first form of (A5). Starting from the formula

$$V^{,\beta}=\bar{V}^{,i}g^{\beta}_{,i}\ , \tag{A10}$$

a special case of (3.15). A straightforward calculation in the tensor calculus yields the result

$$V^{;\beta}_{;\alpha}=\bar{V}^{;i}_{;j}g^{\beta}_{,i}f^{j}_{,\alpha}-\gamma^{i}_{kj}\bar{V}^{,k}g^{\beta}_{,i}f^{j}_{,i}+\bar{V}^{,i}g^{\beta}_{,ij}f^{j}_{,\alpha}+\Gamma^{\beta}_{\sigma\alpha}\bar{V}^{,k}g^{\sigma}_{,k} \tag{A11}$$

and

$$U_{,\alpha}=V^{;\beta}_{;\alpha}V_{,\beta}=V^{;\beta}_{;\alpha}\bar{V}_{,k}f^{k}_{,\alpha}\ . \tag{A12}$$

Comparing (A11) and (A12) with (A7) and (A8), the requirement that they be equal for decoupled motion yield the conditions

$$f^{k}_{,\beta}\bar{V}^{,i}\bar{V}_{,k}(g^{\beta}_{,ij}+\Gamma^{\beta}_{\gamma\alpha}g^{\alpha}_{,i}g^{\alpha}_{,j}-\gamma^{l}_{ij}g^{\beta}_{,l})=0\ . \tag{A13}$$

Using the extended class of point functions defined in Eq. (3.27), we can derive other equations similar to (A13) and differing only in that $\bar{V}^{,i}\bar{V}_{,k}$ is replaced by $\bar{V}^{,i}\bar{U}_{,k}$ and $\bar{U}^{,i}\bar{U}_{,k}$. For the case $K=2$, just as argued in Sec. (III.C), this suffices for us to conclude that

$$f^{k}_{,\beta}\{g^{\beta}_{,ij}+\Gamma^{\beta}_{\gamma\alpha}g^{\gamma}_{,i}g^{\alpha}_{,j}-\gamma^{l}_{ij}g^{\beta}_{,l}\}=0\ . \tag{A14}$$

Actually the derivation can be generalized to any value of K, though we shall continue to discuss the case $K=2$.

To understand the content of Eq. (A14), let us temporarily change subjects. Let λ^1 and λ^2 be parameters (coordinates) defining a surface with covariant metric tensor $\bar{B}_{ij}, i,j=1,2$. The integral of surface area is

$$S_2=\int D_2^{1/2}d\lambda^1 d\lambda^2\ , \tag{A15}$$

where

$$D_2=\begin{vmatrix}\bar{B}_{11} & \bar{B}_{12}\\ \bar{B}_{21} & \bar{B}_{22}\end{vmatrix}=\det\bar{B}_{ij}\ . \tag{A16}$$

From (A15) and (A16), it is a standard calculation to derive the equation of the minimum surface (with fixed boundary), the condition $\delta S_2=0$ yielding the equation

$$\bar{B}^{ij}g^{\alpha}_{,ij}+\bar{B}^{ij}\Gamma^{\alpha}_{\beta\gamma}g^{\beta}_{,i}g^{\gamma}_{,j}-\bar{B}^{ij}\gamma^{k}_{ij}g^{\alpha}_{,k}=0\ . \tag{A17}$$

We finally prove that (A14) implies (A17). First we rewrite (A14) in a set of coordinates adapted to the surface Σ, namely the coordinates q^{μ} such that $q^{a}=0$, $a=3,\ldots,N$ and

$$q^{i}=q^{i}(\lambda^1\lambda^2),\quad i=1,2\ . \tag{A18}$$

In these coordinates (A14) becomes

$$f^{k}_{,l}(g^{l}_{,ij}+\Gamma^{l}_{mn}g^{m}_{,i}g^{n}_{,j}-\gamma^{m}_{ij}g^{l}_{,m})=0\ . \tag{A19}$$

In this case $f^{k}_{,l}$ are the elements of a 2×2 invertible matrix at each point, and so we can conclude that

$$g^{l}_{,ij}+\Gamma^{l}_{mn}g^{m}_{,i}g^{n}_{,j}-\gamma^{m}_{ij}g^{l}_{,m}=0\ . \tag{A20}$$

Next we observe that (A20) is correct, as has just been established, not only for $l=1,2$ but also for $a=3,\ldots,N$, because in this case each term in the equation is zero. This is so for the first and last terms by the choice of q^{μ} and for the middle term because $\Gamma^{a}_{ij}=0$ as a consequence of the decoupling conditions. Altogether, we can therefore write in an arbitrary coordinate system

$$g^{\alpha}_{,ij}+\Gamma^{\alpha}_{\beta\gamma}g^{\beta}_{,i}g^{\gamma}_{,j}-\gamma^{l}_{ij}g^{\alpha}_{,l}=0\ . \tag{A21}$$

Contracting (A21) with $\bar{B}^{ij}$ yields (A17). Thus a decoupled surface must be a geodesic surface as we set out to prove. If the space is Euclidean, exactly decoupled surfaces are planes, as we found directly in the example of Sec. V.

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