Is There a Consistent Theory of Large-Amplitude Collective Motion?

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Villars's equations, first derived from the adiabatic limit of time-dependent Hartree-Fock theory, are presented here as a set of exact conditions for the decoupling (in the adiabatic limit) of a subsystem from a classical Hamiltonian system. It is emphasized that these conditions do not incorporate all the required decoupling conditions. By combining the additional requirements with Villars's equations, we obtain a mathematically complete system, which will yield exact solutions where such exist, but which can also be applied to cases of approximate decoupling.

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A self-consistent theory of large-amplitude collective motion is necessary for a fundamental understanding of a number of prominent features of nuclear collective behavior. Examples are large-amplitude vibrations of transitional nuclei and the coupled rotation-vibrations of deformed nuclei,[1] low-energy fission,[2] and low-energy fusion.[3] Though significant and fruitful efforts to construct a theory have been made for more than a decade, an examination of the proceedings[4] of the last major conference devoted to a review of this subject should convince any reader that the question posed in the title of this Letter remains unresolved.

The purpose of this note is to suggest that a solution to this problem is already inherent in the formulations available in the literature, but that it requires a fresh look at the content of these formulations. Our discussion will be carried out within the framework of classical mechanics in the Hamiltonian form. As shown repeatedly in different guises,[5-8] this should define the leading contributions of the quantum theory even in the nuclear case, where time-dependent Hartree-Fock theory (the most customary starting point) can be written in classical Hamiltonian form.[9,10]

Our precise definition of collective motion is that it is exactly decoupled motion.[11] Limiting ourselves to a Hamiltonian quadratic in the momenta (adiabatic limit), we obtain a set of *exact* conditions for such decoupling, known as Villars's equations.[12,13] At the same time, we demonstrate in physical terms why these are an incomplete description of the system. A set of equations which incorporates the additional requirements is presented and shown to provide, together with Villars's equations, a fully determined theory of decoupled (collective) motion. For the one-dimensional case, it leads to the valley path discussed at length in previous work,[14-19] but for more than one collective degree of freedom our method is new. In the concluding section we describe how the *same equations* may be used to study approximately decoupled motion and how a natural measure of the error of decoupling may be introduced.

Conditions for exactly decoupled motion.—We study a system described by the classical Hamiltonian[20]

$$H(\mathbf{p},\mathbf{x})=\tfrac{1}{2}\sum_{\alpha=1}^{N}p_\alpha^2+V(x_1,\ldots,x_N), \tag{1}$$

containing N pairs of "single-particle" coordinates and momenta, $(x_1,\ldots,x_N)$ and $(p_1,\ldots,p_N)$. We introduce a locally invertible point canonical transformation,

$$x_\alpha=\phi_\alpha(Q_1,\ldots,Q_N), \tag{2}$$

$$p_\alpha=(\partial Q_\mu/\partial x_\alpha)P_\mu, \tag{3}$$

where (3) (sum over μ) is well known from Lagrangean mechanics. We ask for the conditions that a transformation (2) exist such that the transformed Hamiltonian can be separated in at least one way into two noninteracting parts,

$$H(\mathbf{p}(\mathbf{Q},\mathbf{P}),\mathbf{x}(\mathbf{Q}))\equiv\bar{H}(\mathbf{P},\mathbf{Q})=H_C(P_1,\ldots,P_k;\,Q_1,\ldots,Q_k)+H_{\mathrm{NC}}(P_{k+1},\ldots,P_N;\,Q_{k+1},\ldots,Q_N). \tag{4}$$

[Note that from (2) and (3), H_C (the "collective" Hamiltonian) has the form $(i,j=1,\ldots,k)$

$$H_C=\tfrac{1}{2}P_iK^{ij}P_j+\bar{V}(Q_1,\ldots,Q_k), \tag{5}$$

$$K^{ij}=(\partial Q_i/\partial x_\alpha)(\partial Q_j/\partial x_\alpha), \tag{6}$$

with a corresponding expression for H_{NC}.] The dynamical requirements that must be satisfied are simply stated: Any solution of Hamilton's equations for the subsystem described by H_C,

$$\dot{Q}_i = \partial H_C/\partial P_i, \tag{7}$$

$$\dot{P}_i = -\partial H_C/\partial Q_i, \quad i=1,\ldots,k, \tag{8}$$

must also be a solution of the full set of Hamilton's equations for $x_\alpha(\mathbf{Q})$ and $p_\alpha(\mathbf{P},\mathbf{Q})$ when these are restricted initially to the hypersurface Σ, defined by the conditions

$$Q_{k+1}=\ldots=Q_N=P_{k+1}=\ldots P_N=0; \tag{9}$$

i.e., if the system point is initially on Σ, it must remain on Σ.

The consequences of these requirements may be explored within the context of Hamilton's equations of motion for the full system, and one may derive, as has been done several times recently,[10,17,20] a set of conditions which follow from the vanishing of an inhomogeneous polynomial of degree two in the P_i. These equations, given below, refer strictly to the surface Σ. The conditions of degree zero and one are, respectively,

$$\partial V/\partial x_\alpha = (\partial \bar{V}/\partial Q_i)(\partial Q_i/\partial x_\alpha), \tag{10}$$

$$\partial Q^i/\partial x_\alpha = K^{ij}(\partial \phi_\alpha/\partial Q_j). \tag{11}$$

As has been stated repeatedly in the previous work, the condition of second order in P_i is a consequence of (11) and of the kinematical constraint

$$\delta_{ij} = \partial Q_i/\partial Q_j = (\partial Q_i/\partial x_\alpha)(\partial \phi_\alpha/\partial Q_j) \tag{12}$$

[which are a partial set of consequences of (2)]. What has not been appreciated until now is that the proof of this statement entails a decoupling condition not expressed by either Eq. (10) or Eq. (11).[21]

To understand this point, let us list in "raw" form the decoupling conditions implied by the requirements (4) and (5): (i) V separates into two parts, one depending on the Q_i, $i=1,\ldots,k$, and the other on the Q_a, $a=k+1,\ldots,N$. This is the content of Eq. (10). (ii) $K^{ia}=K^{ai}=0$, i.e., the mass tensor has block-diagonal form. This is the content of Eq. (11). (iii) K^{ij} does not depend on Q_a and K^{ab} does not depend on the Q_i, i.e.,

$$\partial K^{ij}/\partial Q_a = \partial K^{ab}/\partial Q_i = 0, \tag{13}$$

$$i,j=1,\ldots,k; \quad a,b=k+1,\ldots,N.$$

The statement made above concerning the dependence of the second-order condition on Eqs. (11) and (12) is true provided that the first of Eqs. (13) is satisfied. This observation, which to our knowledge has not been made previously in the literature, will have a profound effect on understanding finally how to construct a closed theory of large-amplitude collective motion (in the adiabatic limit).

Let us also remark that the distinction made in (4) between collective and noncollective is physical, not mathematical, and therefore our equations, if complete, should provide the possibility of constructing either H_C or H_{NC}. This involves the interchange of the sets i and a and therefore implies that the second of the conditions in (13) must also be considered as a decoupling condition.

Equations (10)–(12) are the Villars equations for the system under study. The problem that we propose to solve in this communication is what conditions have to be adjoined to these equations to fix uniquely the decoupled hypersurface Σ, provided that the latter exists. Our basic idea is the following[22]: Suppose that Σ is k dimensional. Then it can be reconstructed provided that we can specify the tangent plane at each of its points. These are determined by the k tangent vectors $(\partial\phi_\alpha/\partial Q_i)$, $i=1,\ldots,k$. But according to (10) and (11) [$V_\alpha \equiv (\partial V/\partial x_\alpha)$]

$$V_\alpha = (\partial \bar{V}/\partial Q_i)K^{ij}(\partial\phi_\alpha/\partial Q_j) \equiv \lambda^j(\partial\phi_\alpha/\partial Q_j), \tag{14}$$

which implies that the tangent plane must contain a fall line (or line of force) of the potential. If we can find $k-1$ additional vector-valued functions, constructed from the "ingredients" of the Hamiltonian, which satisfy relations of the form (14), we will have satisfied our goal, for altogether we would have a basis for the tangent plane. In fact, we shall go further. We shall exhibit at least $k+1$ such vectors. The requirement of linear dependence among these vectors will determine the hypersurface Σ,

$$x_\alpha = \phi_\alpha(Q_1,\ldots,Q_k). \tag{15}$$

Determination of the collective hypersurface.—The discussion carried out in the previous section suggests that if useful additional equations of the form (14) are to be found, they must incorporate the consequences of (13), which are the only decoupling conditions not so far exploited. We state the relations needed in the form of a theorem, which constitutes the most important new result of this communication: Let us define the family of scalars

$${}^{(1)}V \equiv V, \tag{16}$$

$${}^{(\sigma+1)}V = \tfrac{1}{2}\textstyle\sum_\alpha {}^{(\sigma)}V_\alpha\, {}^{(\sigma)}V_\alpha. \tag{17}$$

Provided that Villars's equations *and* the conditions (13) are satisfied, then ${}^{(\sigma)}V_\alpha$ satisfies an equation of the form

$${}^{(\sigma)}V_\alpha = {}^{(\sigma)}\lambda_j(\partial\phi_\alpha/\partial Q_j). \tag{18}$$

[For $\sigma=1$, we have Eq. (14), and for $\sigma=2$, the result is also well known[16].] The proof of (18), though not

difficult, will not be given here. It can also be shown that the set (18) is only a subset of all scalars whose gradients are tangent to the collective hypersurface. The larger set of scalars consists of the scalar products of *any* previous vectors in the set.

Let us consider briefly (and by example) how Eqs. (18) [in conjunction with Eqs. (10) and (11)] determine a hypersurface Σ and associated quantities. As an illustration, we study the case $N=3$, $k=2$. Without loss of generality,[23] we may choose $x_1=Q_1$, $x_2=Q_2$, and

$$x_3=\phi(x_1,x_2). \tag{19}$$

With this choice of coordinates, the relevant Eqs. (18) can be shown to reduce to the form

$$^{(\sigma)}V_3={}^{(\sigma)}V_1\left(\frac{\partial\phi}{\partial x_1}\right)+{}^{(\sigma)}V_2\left(\frac{\partial\phi}{\partial x_2}\right), \qquad \sigma=1,2,3. \tag{20}$$

The consistency of these equations is possible only if

$$\det|{}^{(\sigma)}V_\alpha|=0, \quad \sigma,\alpha=1,2,3. \tag{21}$$

Since from a given Hamiltonian each element ${}^{(\sigma)}V_\alpha$ can be computed as a function of x_1, x_2, and x_3, the solution of (21) is of the form (19). From (20), the partial derivatives of ϕ are then determined consistently. Finally, returning to Eqs. (11) and (12), the six quantities $(\partial Q_i/\partial x_\alpha)$ can be found easily.

The collective Hamiltonian is computed from the equations

$$\bar{V}(x_1,x_2)=V(x_1,x_2,\phi(x_1,x_2)), \tag{22}$$

$$K^{ij}(x_1,x_2)=(\partial Q_i/\partial x_\alpha)(\partial Q_j/\partial x_\alpha). \tag{23}$$

This method can be extended to any N and any $k<N$. Preliminary calcultations indicate that it is feasible in practice.[24]

Discussion.—In racing through to the final goal, the collective Hamiltonian characterized by (22) and (23), we have left a number of interesting and vital questions behind in the wake: (i) We have assumed an exact decoupling situation. This assumption was made when we directed the reader to calculate the derivatives $(\partial\phi/\partial x_i)$ from (20) when we could equally have made the calculation by differentiation of the solution of (21). When the two methods of calculation agree we have an exactly decoupled situation! (ii) In practice we are more interested in cases of approximate decoupling. Remarkably, the method described is perfectly suited for such a study. If in Villars's equations (11) and (12) and in Eq. (18) we make the replacement

$$\partial\phi_\alpha/\partial Q_i \rightarrow y^i_\alpha, \tag{24}$$

an examination of our algorithm shows that it can be carried through *unchanged.*[25] The listed equations thus determine a hypersurface Σ, Eq. (15), and associate to each point of Σ a plane spanned by the k vectors y^i_α, $i=1,\ldots,k$. For *decoupled motion, these are the tangent planes to* Σ. Otherwise, we may define a natural measure of error at each point: Let

$$\delta^i_\alpha=y^i_\alpha-(\partial\phi_\alpha/\partial Q_i)\equiv y^i_\alpha-\phi^i_\alpha. \tag{25}$$

Then

$$\Delta(Q_1,\ldots,Q_k)=\delta^i_\alpha K^{ij}\delta^j_\alpha/\phi^k_\beta K^{kl}\phi^l_\beta \tag{26}$$

is such a measure. Grosser measures may be introduced by the carrying out of suitable averages of (26). (iii) A word should be said about the geometric significance of the proposed solution. For $k=1$, the equations which replace (21) may easily be shown to be the defining equations for stationary paths (including valleys) on the potential energy surface.[14–19] For $k>1$, it can be argued that Eqs. (21) [or, more generally, (18)] constitute a reasonable definition of a stationary hypersurface on the potential energy surface.[26] (iv) The only alternative method proposed in the literature, applicable to the case $k>1$, is the method described by Rowe and Basserman[9] or by Marumori.[27] It is the *only* method available when the adiabatic approximation is not valid. However, in the adiabatic limit, it is an approximate form of the theory in this paper. For values of k other than 1 or 2, it *may* be more convenient to apply in practice than the exact method, and since one is interested in situations of approximate decoupling anyway, the additional errors thus introduced may not be intolerable [and in any event can be checked by means of (26)]. The questions raised here are matters for future study.

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[20]The close relation of this problem with the nuclear problem is explored most thoroughly in G. Do Dang and A. Klein, University of Pennsylvania Report No. UPR-003NT (to be published).

[21]This point was overlooked in Refs. 10, 17, and 19.

[22]We have recourse to this development because the direct use of (10)–(13) would be clumsy at best, even for exactly decoupled motion. For approximately decoupled motion, it would be quite hopeless.

[23]The decoupling (4) is maintained under any point transformation on Σ. This means that k of the $\phi_\alpha(\mathbf{Q})$ can (in general) be chosen arbitrarily.

[24]G. Do Dang and A. Klein, University of Pennsylvania Report No. UPR-004NT, 1985 (to be published).

[25]For the case of exact decoupling, this algorithm, based on the use of the ${}^{(\sigma)}V$ for the smallest values of σ, can be replaced by equivalent (but less convenient) algorithms with different values of σ. In the approximately decoupled case this is no longer true.

[26]G. Do Dang and A. Klein, University of Pennsylvania Report No. UPR-0014NT, 1985 (to be published).

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