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OPTIMAL OSCILLATION-CENTER TRANSFORMATIONS

By

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## OPTIMAL OSCILLATION-CENTER TRANSFORMATIONS

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## Abstract

A variational principle is proposed for defining that canonical transformation, continuously connected with the identity transformation, which minimizes the residual, coordinate-dependent part of the new Hamiltonian. The principle is based on minimization of the mean-square generalized force. The transformation reduces to the action-angle transformation in that part of the phase space of an integrable system where the orbit topology is that of the unperturbed system, or on primary KAM surfaces. General arguments in favor of this definition are given, based on Galilean invariance, decay of the Fourier spectrum, and its ability to include external fields or inhomogeneous systems. The optimal oscillation-center transformation for the physical pendulum, or particle in a sinusoidal potential, is constructed.

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**MASTER**

## 1. INTRODUCTION

In many areas of classical physics we wish to know the nature of the orbits arising from a Hamiltonian  $H$  of the form  $H_0(p,t) + H_1(q,p,t)$ , where the "unperturbed" Hamiltonian  $H_0$  is a function only of the momentum  $p$  (and possibly of the time  $t$ ), so that the canonical Poisson bracket [1]  $\{p, H_0\}$  vanishes. Thus the unperturbed phase space orbits lie in surfaces of constant  $p$  for all time: the unperturbed system is integrable. The "perturbation"  $H_1$  can have a profound effect on the orbits because it depends on the position  $q$ , so that  $\dot{p} = \{p, H\} \neq 0$ . However, if a canonical transformation [1] to new variables  $Q, P$  can be found such that the new Hamiltonian  $K$  is of the form  $K(P,t)$  [so  $\dot{P} = \{P, K\} = 0$ ], then the perturbed system is also integrable: phase space is filled with invariant surfaces.

Over the past quarter century it has become widely appreciated that real systems are almost never integrable in this strict sense. Yet many systems are "close to integrable." One attempt to make this concept precise was the Kolmogorov-Arnol'd-Moser (KAM) theorem [2], which shows that for sufficiently small and smooth  $H_1$ , invariant surfaces form a set of positive measure. It is the goal of this paper to suggest a possible way to interpolate between the KAM surfaces, and to extrapolate past their breakup as the perturbation is increased by defining an optimization criterion for canonical transformations.

We call optimal, close-to-KAM coordinates "oscillation-center (OC) coordinates" provided the transformation also satisfies the topological constraint of continuous connection with the identity transformation (i.e., it is the limit of a sequence of diffeomorphisms). This means that the surfaces of constant OC momentum can at best be primary KAM surfaces, i.e., those which have the same topology as the invariant surfaces of the unperturbed system. To try to capture higher order KAM surfaces would lead to a transformation so

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complicated that one could not hope to prescribe a simple algorithm for its computation. Thus, in general, an OC transformation cannot effect a complete integration, even of an integrable system. Its purpose is simply to provide orbit coordinates that are always close to the original coordinates, yet which have as constant momenta as possible. The difference between these coordinates and the original ones will oscillate with time in a nonsecular fashion, hence the name "oscillation-center coordinates."

Oscillation-center transformations have proved useful in the understanding of ponderomotive force effects in plasmas [3-7] and show promise of providing a better description of particle motion in turbulent plasmas [8,9]. Another important potential application is in the choice of the optimal coordinates for the description of three-dimensional magnetic field configurations in plasma containment devices. Any toroidal magnetic field [10]  $\underline{B}$  can be represented as

$$\underline{B} = \underline{\nabla}\zeta \times \underline{\nabla}\Psi(\phi, \theta, \zeta) + \underline{\nabla}\phi \times \underline{\nabla}\theta$$

where  $\zeta$  is a toroidal angle,  $\theta$  is a poloidal angle, and  $\phi$  and  $\Psi$  are toroidal and poloidal flux functions, respectively. It is clear that the field lines obey Hamiltonian equations of motion if  $\zeta$  is interpreted as a "time" and  $\Psi$  as a Hamiltonian, with  $\theta$  and  $\phi$  being conjugate position and momentum variables. The transformation to the magnetic coordinates widely used for plasma equilibrium and stability calculations can be viewed [11,12] as an action-angle transformation to a new Hamiltonian  $\Psi(\phi)$ , if it exists. Such a transformation exists only if the original Hamiltonian is integrable, which is true generally only if the system possesses a continuous symmetry [13].

Thus we need to find a best approximation to magnetic coordinates in

nonsymmetric systems. This is identical with the oscillation-center problem. A method has been proposed by Boozer [14] based on Fourier analysis of the fluctuations of the coordinates of a point following a field line. This has worked well on vacuum fields produced by prescribed conductors, and has been extensively developed and automated [15]. Nevertheless, a certain amount of subjectivity remains both in the choice of starting points for the line tracing when magnetic islands are present, and in the assignment of an amplitude to broadened and distorted Fourier peaks arising when non-KAM behavior occurs.

In finite- $\beta$  plasma equilibrium calculations the choice of coordinate is more intimately involved with the actual computation of the magnetic field itself. In several recent approaches [16-19] the coordinate system is chosen dynamically to minimize the residual errors. These methods are tied to the assumption of perfect magnetic (KAM) surfaces, but are interesting in that they demonstrate that modern computers are capable of accurately minimizing a complicated nonlinear functional (the total energy) over a multidimensional trial function space. This suggests that the use of a subsidiary variational principle to optimize the more general (and therefore less unique) representation needed to represent equilibria with imperfect magnetic surfaces should be computationally feasible, and may be more efficient and easier to automate than the field-line tracing method.

In Sec. 2 we discuss two possible variational principles for defining the optimal OC transformation. The first minimizes a functional  $I_0$  containing no derivatives of the Hamiltonian  $K$ , and can produce a Hamiltonian with jumps. We call this transformation the  $OC^{-1}$  transformation. The second principle minimizes a functional  $I_1$  quadratic in the first derivatives of  $K$  with respect to the new position coordinates. Thus  $K$  must be a continuous ( $C^0$ ) function of

position. We call this the  $OC^0$  transformation.

In Sec. 3 we demonstrate the Galilean invariance of  $I_1$ , and also show that the  $OC^0$  Hamiltonians must have a Fourier spectrum decaying at least as fast as  $|k|^{-3/2}$ , and that the minimization of  $I_1$  naturally allows external fields or inhomogeneities to be incorporated in the OC formalism.

In Sec. 4 we derive the Euler-Lagrange equation for extrema of  $I_1$ , and suggest a method for its minimization by the method of steepest descents. In Sec. 5 we solve the Euler-Lagrange equation for the case of the physical pendulum, and in Sec. 6 we speculate on the properties of the  $OC^0$  Hamiltonian in nonintegrable systems.

## 2. VARIATIONAL PRINCIPLES

A variational principle for optimizing OC transformations has been suggested by Dewar [20] based on the minimization of

$$I_0 \equiv \int d^N P \langle [K(Q, P, t) - \bar{K}(P)]^2 \rangle \quad (2.1)$$

where  $\langle \rangle$  denotes averaging over  $Q$  and  $t$  at constant  $P$ ,  $\bar{K} \equiv \langle K \rangle$ , and  $N$  is the number of degrees of freedom. The optimal transformation for the physical pendulum Hamiltonian

$$H = \frac{P^2}{2} - \cos \theta \quad (2.2)$$

(in suitable units) was constructed. However, the resulting transformation (we shall call this the  $OC^{-1}$  transformation) is highly discontinuous, though it is the limit of a sequence of continuous transformations, and no practical way to treat more general cases has been found.

It is possible that the discontinuous transformation can be associated with the branch cuts of the analytic continuation of the standard action-angle transformation, for rotational motion, around the branch point at  $J = \pm J_S$ , where

$$J_S = \frac{4}{\pi} \tag{2.3}$$

is the action at the separatrix between rotational and libratory motion, but even for the physical pendulum the analytic structure of the action-angle transformation is very complicated [21]. In nonintegrable systems the situation is much worse [22]. Thus even renormalized perturbation theory cannot hope to treat this kind of transformation, and the discontinuous nature of the mapping makes numerical methods difficult, too.

Clearly we need a variational principle which produces a smoother transformation. If we consider a hierarchy of variational principles, producing Hamiltonians which are smoother and smoother in the  $Q$  coordinates, the transformation just described is the lowest member. In this paper we consider the next member of the hierarchy: that transformation (the  $QC^0$  transformation) which minimizes

$$I_1 \equiv \frac{1}{2} \int d^N P \sum_{i=1}^N [ \langle \{K, P_i\}^2 \rangle - \langle K, P_i \rangle^2 ] \tag{2.4}$$

where we define the averaging by

$$\langle * \rangle \equiv \int_{-T/2}^{T/2} T^{-1} dt \int_{-L_1/2}^{L_1/2} L_1^{-1} dQ_1 \dots \int_{-L_N/2}^{L_N/2} L_N^{-1} dQ_N * \tag{2.5}$$

with  $T, L_1, \dots, L_N$  being the periodicity scales of the system, or large



intervals tending to infinity. The second term in (2.4) vanishes for quasi-periodic Hamiltonians, but is needed for systems with external fields (see later).

Since  $\{K, P_i\} = \partial K / \partial Q_i$ ,  $K$  must be at least continuous in  $Q$  for  $I_i$  to exist. Where primary KAM surfaces exist, (2.4) clearly will select a transformation such that  $\{K, P_i\} = 0$ , as desired. Elsewhere, the mean-square generalized force  $-\{K, P_i\}$  is minimized. One suspects that trying to demand higher continuity with respect to the  $Q$ -dependence would lead to less continuity with respect to the  $P$ -dependence. At any rate the  $OC^0$  transformation seems the simplest and most practical and we devote the remainder of this paper to its study.

### 3. PROPERTIES OF THE $OC^0$ TRANSFORMATION

#### A. Galilean Invariance:

Since the  $OC$  coordinates must, on average, follow the original coordinates, they must transform the same way as the original coordinates under Galilean transformation. The requirement that the momenta must be canonically conjugate to the coordinates then means that the  $OC$  momenta must also transform the same way as the original momenta. For simplicity we consider a single particle whose Cartesian  $OC^0$  variables are  $\tilde{x}^0$  and  $\tilde{p}^0$  in some frame moving with velocity  $\underline{v}$  with respect to the laboratory frame. The corresponding laboratory frame variables are then given by

$$\tilde{p} = \tilde{p}^0 + \underline{v} ,$$

$$\tilde{x} = \tilde{x}^0 + \underline{v}t . \tag{3.1}$$

The generating function [1] for this transformation is

$$F(\underline{X}^0, \underline{P}) = (\underline{X}^0 + \underline{V}t) \cdot (\underline{P} - \underline{V}) . \quad (3.2)$$

Thus the Hamiltonian transforms according to

$$K(\underline{X}, \underline{P}, t) = K^0(\underline{X}^0, \underline{P}^0, t) + \underline{V} \cdot \underline{P}^0 . \quad (3.3)$$

From the invariance of Poisson brackets and phase-space volumes under canonical transformations it now readily follows that  $I_1$  is invariant under Galilean transformations. This is a persuasive argument in favor of minimizing  $I_1$ , rather than a functional involving time derivatives.

#### B. Fourier Spectrum:

Let

$$K = \sum_{\underline{k}} K_{\underline{k}}(\underline{P}, t) \exp(i\underline{k} \cdot \underline{X}), \quad (3.4)$$

then

$$\langle |K(\underline{k}, \underline{P})|^2 \rangle = \sum_{\underline{k}} |\underline{k}|^2 \langle |K_{\underline{k}}|^2 \rangle . \quad (3.5)$$

If we suppose that  $\langle |K_{\underline{k}}|^2 \rangle^{1/2}$  is proportional to  $|\underline{k}|^{-\alpha}$  at large  $|\underline{k}|$ , then (3.5) implies that

$$\alpha > 3/2 \quad (3.6)$$

for  $I_1$  to exist. Thus, although  $K_k$  is not guaranteed to have exponential decay, the Fourier coefficients must decay reasonably rapidly. In a practical application of the variational principle, where a finite number of smooth trial functions were used, the resulting transformation would be suboptimal, but smoother, and therefore lead to a more rapidly decaying  $K_k$  spectrum (assuming  $H$  smooth).

C. External Fields:

Consider the Hamiltonian for a particle of charge  $e$  in an external electric field  $\underline{E} = \underline{E}_0 - \nabla\phi(\underline{x}, t)$ , where  $\underline{E}_0$  is constant,

$$H = \frac{p^2}{2m} + e\phi(\underline{x}, t) - e\underline{x} \cdot \underline{E}_0 . \quad (3.7)$$

The presence of the last term in (3.7) precludes the possibility of finding a new Hamiltonian of the form  $K(\underline{p}, t)$ , since the transformation would be singular as  $|\underline{x}| \rightarrow \infty$ . Thus the best we can hope for is

$$K = K_0(\underline{p}, t) - e\underline{x} \cdot \underline{E}_0 . \quad (3.8)$$

In ponderomotive force problems [7] we also want Hamiltonians whose  $X$  dependence is approximately linear over the scale of a wavelength.

We now demonstrate that minimization of  $I_1$  will naturally select Hamiltonians with linear  $\underline{x}$ -dependence, provided this is consistent with the topological constraints. It is easily shown that

$$I_1 > 0 , \quad (3.9)$$

with equality if and only if

$$\{K, P_i\} = \text{const}, \tag{3.10}$$

which implies that K is a linear function of the  $Q_i$ , as desired. This does not occur so naturally if we minimize  $I_0$ .

#### 4. MINIMIZATION OF $I_1$

The functional  $I_1$ , (2.4), is to be minimized under the constraint that the variations are canonical. This can be ensured by using an infinitesimal generator  $\delta G = W(Q,P,t,\epsilon)\delta\epsilon$  such that

$$\delta z = \{z, W\} \delta\epsilon, \tag{4.1}$$

where z is any of the phase space coordinates  $q_i$  or  $p_i$  expressed as functions of Q, P, t, and  $\epsilon$ . The variation in K is given by [9,20]

$$\delta K = -(\partial_t + L_K) W \delta\epsilon \tag{4.2}$$

where the Liouville operator  $L_K$  is defined by

$$L_K * \equiv \{*, K\}, \tag{4.3}$$

and  $\partial_t$  denotes  $\partial/\partial t$ .

Using (4.2), we find, after integration by parts

$$\delta I_1 = -\delta\epsilon \int d^N P \langle W (\partial_t + L_K) \nabla^2 K \rangle, \tag{4.4}$$

where

$$\nabla^2 K \equiv \sum_{i=1}^N \frac{\partial^2 K}{\partial Q_i^2}, \quad (4.5)$$

and we have assumed that  $W \rightarrow 0$  as  $|P_i| \rightarrow \infty$ , and that  $W$  remains finite as  $T$  and the  $L_i$  in the averaging operation  $\langle \rangle$  defined in (2.5) tend to infinity, so that the endpoint contributions vanish in this limit. If  $T$  and  $L_i$  are periodicities, we assume  $W$  to have the same periodicities, so that again there are no endpoint contributions to (4.4).

The condition that

$$\delta I_1 = 0 \quad (4.6)$$

for all  $W$  yields the Euler-Lagrange equation

$$(\partial_t + L_K) \nabla^2 K = 0, \quad (4.7)$$

which is a statement that  $\nabla^2 K$  is a constant of the motion.

In an integrable system we could express  $\nabla^2 K$  in terms of the actions, and then solve for  $K$ . This is essentially the procedure adopted in the next section, where we construct the  $OC^0$  transformation for the physical pendulum. On a primary KAM surface, of course, we set  $\partial K / \partial Q_i = 0$ , so that  $\nabla^2 K$  trivially satisfies (4.7), being identically zero. In a chaotic region of a nonintegrable system, the situation is far less clear, since no simple constants of the motion exist.

We have not yet constructed an  $OC^0$  transformation for a nonintegrable system, but we close this section with a suggested method for numerical

investigation of this problem. The method is that of steepest descents minimization of  $I_1$ . We construct the transformation as the  $\epsilon \rightarrow \infty$  limit of a Hamiltonian flow, with  $W$  playing the role of the Hamiltonian, and  $\epsilon$  that of the time. By choosing

$$W = (\partial_t + L_K) \nabla^2 K \quad , \quad (4.8)$$

we see from (4.4) that

$$\frac{dI_1}{d\epsilon} = - \int d^N P \langle [(\partial_t + L_K) \nabla^2 K]^2 \rangle < 0 \quad , \quad (4.9)$$

with equality applying if and only if (4.7) is satisfied. This is similar to the method [16,17] which has been used to construct numerical hydromagnetic equilibria, and should be feasible to implement for systems with a small number of degrees of freedom, such as the magnetic field in three-dimensional hydromagnetic equilibrium configurations. With results from low dimensional systems as a guide, one hopes to develop general analytical techniques for estimating the statistical behavior of the chaotic part of  $K$ .

## 5. THE PHYSICAL PENDULUM

We start with the Hamiltonian given by (2.2). This Hamiltonian is an important one in plasma physics, because it is the Hamiltonian for a single particle moving in the field of an electrostatic wave, as seen in a frame moving with the phase velocity of the wave. It is also important for the general understanding of phase space islands in Hamiltonian systems as it forms an approximation to the local behavior of a general Hamiltonian in the neighborhood of a resonance when expressed in appropriate canonical

coordinates [23].

We shall denote the  $OC^0$  position and momenta by  $\Theta$  and  $J$ , respectively. For rotational motion these are identical to the standard angle and action [23], and (4.7) is solved trivially by  $K = K(J)$ , where  $K(J)$  is defined implicitly, for  $|J| > J_s$ ,  $K > 1$ , by

$$J = \pm J_s k^{-1} E(k), \quad (5.1)$$

where  $J_s$  is defined by (2.3) and  $E$  is the complete elliptic integral of the second kind [24] with modulus  $k$  given by

$$k^2 = 2/(K + 1). \quad (5.2)$$

Within the separatrix ( $|J| < J_s$ ,  $K < 1$ ) the topological restriction on  $OC$  transformations of continuous connection with the identity forces us to consider solutions of the form  $K = K(O, J)$ , so that the orbits can remain topological circles. However, we can write down the general, time-independent first integral of (4.3) as

$$\partial^2 K / \partial O^2 = -U'(K), \quad (5.3)$$

where  $U'$  is a function to be determined from the global topological and periodicity constraints.

Equation (5.3) was obtained by integrating along the characteristics of the operator  $L_K$ , that is along all the libratory orbits. Its domain of validity is thus the interior of the separatrix,  $-1 < K < 1$ . There are no derivatives with respect to  $J$  remaining, so we can construct the general

solution of (4.7) by integrating (5.3) along lines of constant  $J$  in the interval  $-J_S < J < J_S$ . In fact (5.3) is just the equation for a nonlinear oscillator with  $K$  playing the role of position,  $Q$  the role of time, and  $U$  that of a potential energy function. The topological constraint on the OC transformation means that each line of constant  $J$  in the interval  $-J_S < J < J_S$  must cross the separatrix, where  $K = 1$ . Yet everywhere else on  $J = \text{const}$ , we must have  $K < 1$ . Thus the potential function  $U$  must have a step of sufficient height at  $K = 1$  to act as a barrier which "reflects" the solution back into the region  $K < 1$ . We also require  $K$  to be  $2\pi$ -periodic in  $Q$  for all  $J$ , so that the periods of the motions in the potential  $U$  must be independent of amplitude. This condition uniquely implies a harmonic oscillator potential, so

$$U(K) = \begin{cases} \frac{\infty}{8} & \text{for } K \{ \begin{matrix} > 1 \\ < 1 \end{matrix} \end{cases} , \quad (5.4)$$

where the spring constant has been chosen to give  $2\pi$ -periodic motion in  $Q$ . The general solution of (4.7) consistent with the topological constraints in the libratory region,  $|J| < J_S$ , is thus

$$K = 1 - \Delta(J) |\cos(Q/2)| , \quad (5.5)$$

where we must now determine  $\Delta(J)$  by solving a kind of Hamilton-Jacobi problem for the generating function of the  $OC^0$  transformation.

Rather than transform directly from the  $\theta, p$  representation to the  $Q, J$  representation, we go via the standard action-angle representation  $\hat{Q}, \hat{J}$ , say, in which we denote the Hamiltonian by  $E(\hat{J})$ . Regarding  $\hat{Q}$  and  $\hat{J}$  as the "old" variables, and  $Q$  and  $J$  as the "new" variables, we use a generating function of



the fourth type [1, 23]  $F(J, \hat{J})$  such that

$$0 = \partial F / \partial J, \quad (5.6)$$

$$\hat{0} = -\partial F / \partial \hat{J}, \quad (5.7)$$

and keep the transformation single valued by restricting attention to the first quadrant in the  $0, J$  plane:  $0 > \hat{0} > -\pi/2$ . On an orbit,  $E(\hat{J}) = \text{const}$ , the corresponding domain of  $J$  is  $0 < J < J_0(E)$ , and range of  $0$  is  $0_0(E) > 0 > 0$ , where  $J_0(E)$  and  $0_0(E)$  are intersections of the orbit with the positive  $J$  and  $0$  axes, respectively.

Solving (5.5) for  $0$  and using (5.6) we find the Hamilton-Jacobi type equation

$$\frac{\partial F}{\partial J} = 2 \arccos \frac{1 - E}{\Delta(J)}. \quad (5.8)$$

Integrating (5.8), and substituting in (5.7) we have

$$\hat{0} = -2\mu(\hat{J}) \int_0^J \frac{dJ' / \Delta(J')}{[1 - (1 - E)^2 / \Delta^2(J')]^{1/2}}, \quad (5.9)$$

where

$$\mu(\hat{J}) \equiv \frac{\partial E}{\partial \hat{J}} \quad (5.10)$$

is the angular frequency. By evaluating (5.9) at  $J = J_0(E)$ , and changing the independent variable from  $J$  to  $\Delta$  we find the integral equation for  $J(\Delta)$

$$\int_0^{1-E} \frac{d\Delta J'(\Delta)}{[\Delta^2 - (1-E)^2]^{1/2}} = \frac{T(E)}{8} \quad (5.11)$$

where  $T(E) \equiv 2\pi/\Omega(J)$  is the period of the pendulum. By writing  $y = \Delta^2$ ,  $\tau_1 = (1-E)^2$ , we recognize (5.11) as a convolution equation, which can be solved by Laplace transform to give

$$J(\Delta) = \frac{1}{4\pi} \int_{-1}^{1-\Delta} \frac{(1-E) T(E) dE}{[(1-E)^2 - \Delta^2]^{1/2}} \quad (5.12)$$

That this is the solution may readily be verified by substituting (5.12) into (5.11). We extend the solution to  $J < 0$  by observing that symmetry about  $J = 0$  requires  $\Delta(J)$  to be an even function.

The period is given in terms of the complete elliptic function of the first kind  $K(k)$  by [23]

$$T = 4 K(k) \quad , \quad (5.13)$$

where

$$k = \frac{(1+E)^{1/2}}{2} \quad , \quad (5.14)$$

so that  $1 - E = 2k'^2$ , where  $k'^2 \equiv 1 - k^2$  in the usual way [24].

Defining  $\ell'$  by  $\Delta \equiv 2\ell'^2$ , and  $\ell$  by  $\ell^2 \equiv 1 - \ell'^2$ , we can write (5.12) as

$$J(\ell) = \int_0^{\ell} \frac{k'^2 K(k) dk}{(k'^4 - \ell'^4)^{1/2}} \quad (5.15)$$

Integration by parts yields an expression convenient for expanding about  $\ell = 0$

$$J(\ell) = \ell(2-\ell^2)^{1/2} + \frac{J_s}{2} \int_0^\ell (k'^4 - \ell'^4)^{1/2} \frac{\tilde{K}}{dk} dk, \quad (5.16)$$

hence we find an expression good for  $|J| \ll J_s$

$$\Delta = 2 - J^2 - \frac{J^4}{12} + O(J^6). \quad (5.17)$$

For numerical work, and to expand  $\Delta$  near the separatrix, we transform to a new independent variable  $x$  defined by

$$k' = [(1-\ell'^4)x^2 + \ell'^4]^{1/4}, \quad (5.18)$$

so that

$$J(\ell) = \frac{1}{2} J_s (1-\ell'^4)^{1/2} \int_0^1 \tilde{K}'[k'(x)] dx, \quad (5.19)$$

where  $\tilde{K}'(k) \equiv \tilde{K}(k')$ . For  $J_s - |J| \ll J_s$  we find

$$\Delta = 4(J_s - |J|) + 0 \left[ (J_s - |J|)^2 \ln(J_s - |J|) \right]. \quad (5.20)$$

Numerical evaluation of (5.19) yields the curve plotted in Fig. 1. Level surfaces of  $K$  (orbits in the  $OC^0$  representation) are plotted in Fig. 2. We see that the separatrix has been squeezed into a rectangular shape, with the unstable X-type fixed points being replaced by T-type fixed points. The potential wells are separated by a crease where  $\partial K/\partial \theta$  is discontinuous, as  $\partial K/\partial J$  is discontinuous at  $|J| = J_s$ , but the orbits themselves are all smooth in contrast to the discontinuous motions in the  $OC^{-1}$  representation [20].

The  $OC^0$  mapping does have singularities on the separatrix, however, which suggests that a suboptimal transformation would be better in practice. This is partly an artifact of looking at an integrable system, since sharp separatrices do not exist in the nonintegrable case. Expanding about the stable fixed point at the bottom of a well, we find

$$K = 1 + \frac{1}{4} Q^2 + J^2 + O(Q^4, J^4) \quad (5.21)$$

This is to be compared with the  $(q^2 + p^2)/2$  behavior of  $H$ . Thus the  $OC^0$  transformation has flattened the orbits at the bottoms of the wells from circles into 2:1 ellipses (preserving their periods, of course).

## 6. DISCUSSION

We have found a variational principle which appears to have the properties needed for extending the notion of oscillation-center coordinates to nonintegrable systems, although considerable further investigation is needed to determine whether the problem really is well posed, and whether the resulting transformation is useful for setting up magnetic coordinates or for plasma turbulence problems.

From the example of the physical pendulum worked out in Sec. 5 we observe an interesting interplay of characteristic directions: to obtain (5.3) we integrated along the physical orbits, to obtain (5.5) we integrated along the lines  $J = \text{const}$ , (which are not orbits), and to obtain (5.9) we again integrated along the orbits ( $\hat{J} = \text{const}$ ). This coexistence of characteristic directions suggests that a Lagrangian variational principle of the type used effectively to find KAM surfaces [22, 25, 26] cannot generalize beyond KAM

surfaces since its characteristic directions are defined by the orbits. One can attempt to get around this by modifying the Lagrangian used for constructing the transformation, but there seems to be considerable arbitrariness in how to perform this modification.

On the subject of the utility of the  $OC^0$  transformation to describe chaotic orbits, we permit ourselves a speculation. We can formally integrate (4.7) in terms of the  $Q_i$  and  $P_i$  at some initial time, but the exponential divergence [23] of initially close orbits means that the  $Q$ -dependence of  $K$  will itself be "chaotic," with autocorrelation time determined by the maximum Liapunov exponent [23] for the exponential divergence of trajectories, since  $K$  will "forget" the initial state over this time. That is, the  $OC^0$  transformation will retain an irreducible, chaotic "interaction" part of the Hamiltonian whose statistical properties are intrinsic to the predictability of the orbits rather than to the statistical properties of the original Hamiltonian  $H$ . This allows us to sharpen up somewhat a previous speculation [20] that the  $OC$  transformation will make a Markovian description of the particle orbits more valid: a Markovian approximation for the wave-particle collision operator in the  $OC^0$  representation will be valid provided the distribution function changes on a time scale long compared with the minimum time scale for exponential divergence of trajectories.

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REFERENCES

- [1] H. Goldstein, *Classical Mechanics* (Addison Wesley, Reading, Massachusetts, 1950).
- [2] V.I. Arnol'd and A. Avez, *Ergodic Problems of Classical Mechanics* (Benjamin, New York, 1968).
- [3] G. Schmidt, *Physics of High Temperature Plasmas* (Academic, New York, 1979), 2nd ed. p. 47.
- [4] R.L. Dewar, Interaction Between a Hydromagnetic Wave and a Time-Dependent Inhomogeneous Medium, *Phys. Fluids* 13 (1970) 2710.
- [5] R.L. Dewar, A Lagrangian Theory for Nonlinear Wave-packets in a Collisionless Plasma, *J. Plasma Phys.* 7 (1972) 267.
- [6] R.L. Dewar, Energy-Momentum Tensors for Dispersive Electromagnetic Waves, *Aust. J. Phys.* 30 (1977) 533.
- [7] J.R. Cary and A.N. Kaufman, Ponderomotive Effects in Collisionless Plasma: A Lie Transform Approach, *Phys. Fluids* 24 (1981) 1238.
- [8] R.L. Dewar, Oscillation-Center Quasilinear Theory, *Phys. Fluids* 16 (1973) 1102.
- [9] R.L. Dewar, Renormalized Canonical Perturbation Theory for Stochastic Propagators, *J. Phys. A* 9 (1976) 2043.
- [10] A.H. Boozer, Evaluation of the Structure of Ergodic Fields, *Phys. Fluids* 26 (1983) 1288.
- [11] R.G. Littlejohn and J.R. Cary, Noncanonical Hamiltonian Mechanics and its Application to Magnetic Field Line Flow, *Ann. Phys.* 151 (1983) 1.
- [12] A.H. Boozer, Magnetic Field Line Hamiltonian, Princeton Plasma Physics Laboratory Report PPPL-2094 (1984).
- [13] R.L. Dewar, D.A. Monticello, and W.N.-C. Sy, Magnetic Coordinates for Equilibria with a Continuous Symmetry, *Phys. Fluids* (1984) in press.
- [14] A.H. Boozer, Establishment of Magnetic Coordinates for a Given Magnetic Field, *Phys. Fluids* 25 (1982) 520; Practical Evaluation of Action-Angle Variables, Princeton Plasma Physics Laboratory Report PPPL-2082 (1984).
- [15] G. Kuo-Petravic, A.H. Boozer, J.A. Rome, and R.H. Fowler, *J. Comput. Phys.* 51 (1983) 261.
- [16] F. Bauer, O. Betancourt, and P. Garabedian, A Computational Method in Plasma Physics (Springer-Verlag, New York, 1978); *Phys. Fluids* 24 (1981) 48.

- [17] S.P. Hirshman and J.C. Whitson, Steepest-Descent Moment Method for Three-Dimensional Magnetohydrodynamic Equilibria, *Phys. Fluids* 26 (1983) 3553.
- [18] A. Bhattacharjee, J.C. Wiley, and R.L. Dewar, Variational Method for Three-Dimensional Toroidal Equilibria, *Comp. Phys. Commun.* 31(1984) 213.
- [19] L.L. Lao, J.M. Greene, T.S. Wang, F.J. Helton, and E.M. Zawadzki, Three Dimensional Toroidal Equilibria and Stability by a Variational Spectral Method, GA Technologies Report GA-A17194 (1983).
- [20] R.L. Dewar, Exact Oscillation-Centre Transformation, *J. Phys. A* 11 (1978) 9.
- [21] E. Rosengaus, Renormalization of Perturbation Theories for Action-Angle Transformations, Princeton University Ph.D. Thesis, 1982.
- [22] E. Rosengaus and R.L. Dewar, Renormalized Lie Perturbation Theory, *J. Math. Phys.* 23 (1982) 2328.
- [23] A.J. Lichtenberg and M.A. Lieberman, *Regular and Stochastic Motion* (Springer-Verlag, New York, 1983).
- [24] I.S. Gradshteyn and I.W. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965), pp. 904-905.
- [25] I.C. Percival, A Variational Principle for Invariant Tori of Fixed Frequency, *J. Phys. A* 12 (1979) L57.
- [26] J.M. Greene and I.C. Percival, Hamiltonian Maps in the Complex Plane, *Physica* 3D (1981) 530.



FIGURE CAPTIONS

- Fig. 1. The function  $\Delta(J)$  occurring in the oscillation-center ( $OC^0$ ) Hamiltonian  $K = 1 - \Delta(J) |\cos Q/2|$  for libratory orbits of the physical pendulum.
- Fig. 2. Level curves of oscillation-center ( $OC^0$ ) Hamiltonian  $K$  for the physical pendulum. The rotational orbits are shown as solid lines, while the libratory orbits are dotted. Here  $J_s \equiv 4/\pi$  is the action at the separatrix.

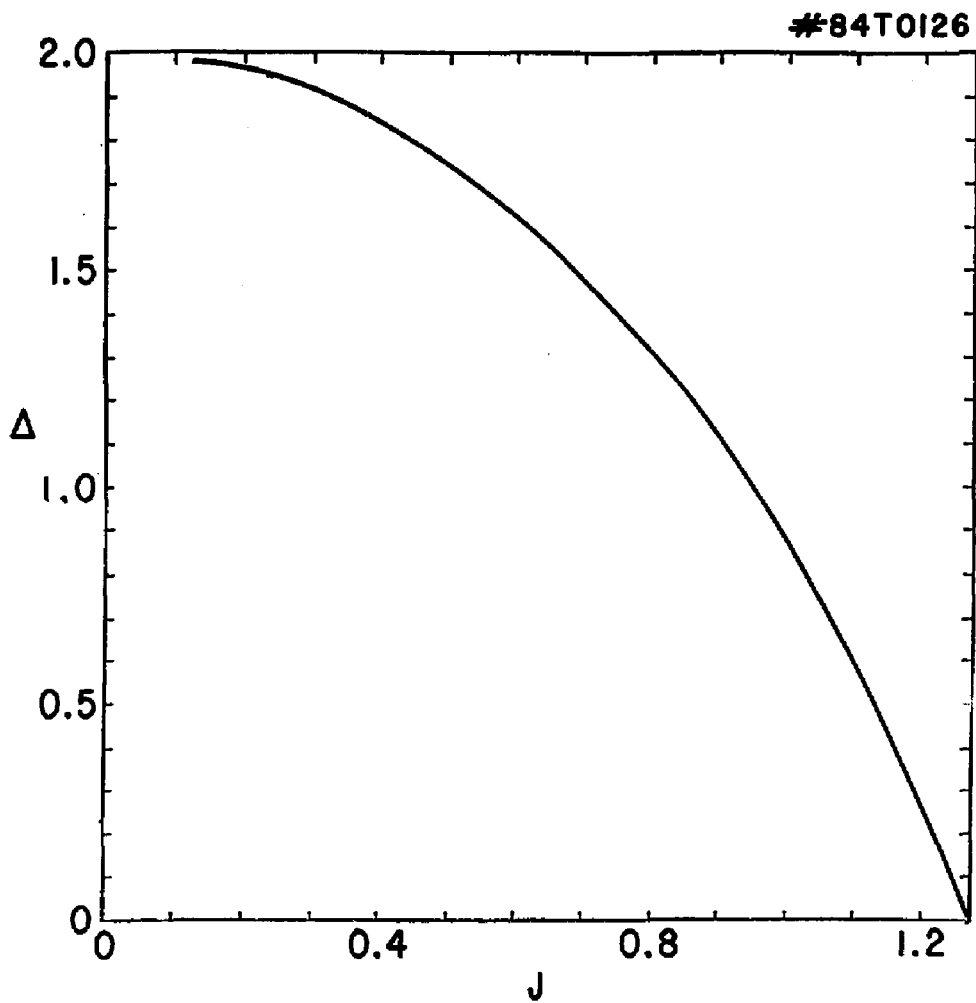


Fig. 1

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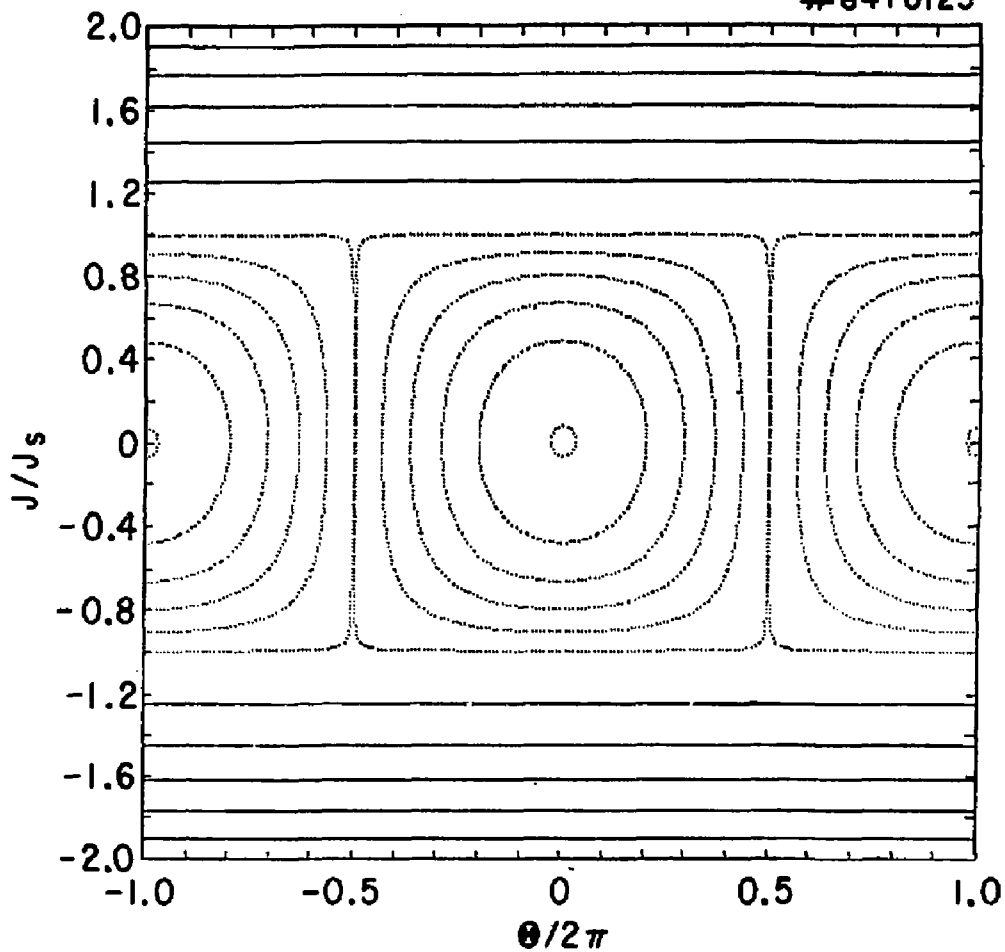


Fig. 2