Predicting Two Dimensional Hamiltonian Chaos *

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We use geometrical analysis to show that the Toda-Brumer-Duff criterion for transition to chaos is a simple application of Jacobi's equation. Further, we propose a new criterion for this transition for two-dimensional hamiltonian systems and summarize the results.

It is well-known [1] that non-linear Hamiltonian systems exhibit a transition from regular to stochastic behaviour with variation of system parameters, especially energy; this is of relevance both in understanding the foundations of statistical mechanics [2], and in the study of chemical kinetics [3]. Even though it has been argued that in such systems, chaotic orbits exist in the phase space for all values of the energy, phenomenologically there is a clear, usually abrupt and phase-transition-like change from smooth curves on Poincaré sections to a random scatter of points [1–5, 7, 8]. Finding this point of transition, or even confirming its existence or lack thereof is both tedious and suspect if done numerically. There have been attempts to find an analytic predictor of the transition energy: principally those of Chirikov, Greene and Mo [6] and, of concern to us here, of Toda [7], Brumer and Duff [8] (herinafter TBD).

We present here a geometrical analysis, both of a 2-d manifold M embedded in $\mathbf{R}^3$ defined by the Monge patch $\mathbf{u} = (x, y, V(x, y))$, and of the contour lines of the potential $V(x, y)$ on the x, y plane to study the transition to (existence of) stochastic behaviour for Hamiltonians of the form

$$H = \frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y} + V(x, y) . \quad (1)$$

Let there be [9] geodesics σ, σ^1 passing through a point p on M. If we set up a polar coordinate system at p, with arc-length r measured along the geodesics and angle ϕ defined by the initial angle between, them, then the line element on M can be written as

$$\mathrm{d}s^2 = \mathrm{d}r^2 + G\,\mathrm{d}\phi^2 , \quad (2)$$

and the Gaussian curvature K as

$$K = -\frac{1}{\sqrt{G}} \frac{\partial^2 \sqrt{G}}{\partial r^2} . \quad (3)$$

If the distance r along σ and σ^1 is the same, the geodesic deviation, $\eta = \sqrt{G}\,\mathrm{d}\phi$ and thence,

$$\eta'' + K\eta = 0 , \quad (4)$$

which is the well-known Jacobi's equation. (This equation can be extended [10] to arbitrary dimensions.) By inspection, for K positive, η has oscillatory solutions, for K negative, exponential solutions. In general, of course, $K = K(x, y)$ and the solutions are non-trivial.

There is a comprehensive discussion in both the works by Arnol'd [10, 11] on the applications and extensions of this by the Russian dynamical systems school, from which we quote: "the exponential instability of geodesics on manifolds of negative curvature leads to the stochasticity of the corresponding geodesic flow." A careful consideration of the TBD criterion shows that it consists of projecting the region of negative Gaussian curvature of the potential manifold onto the energy contours to pick out E_c, the energy of transition, a very straightforward application of Jacobi's equation.

This technique has, with a mixed degree of success, been applied to various 2-d Hamiltonians (see Table 1).

Churchill, Pecelli and Rod studied [12] the function

$$\beta' = V_{xx} V_y^2 + V_{yy} V_x^2 - 2 V_x V_y V_{xy} \quad (5)$$

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Table 1. Critical energies and comparisons with TBD and Numerical values. An ∞ indicates an integrable system.

Name	Potential	E_c (TBD)	E_c (PS)	E_c (Num)
Henon-Heiles [4]	$\frac{1}{2}(x^2+y^2)+\frac{1}{3}x^3-xy^2$	0.0833	0.0833	0.0833
Barbanis [5]	$0.05\,(x^2+y^2)-0.1\,x_y^2$	0.00625	0.0056	0.005+
Toda [7]	$\exp(-y)+\exp(y-x)+\exp(x)-3$	∞	∞	∞
Anti-Henon-Heiles [14]	$\frac{1}{2}(x^2+y^2)+\frac{1}{3}y^3+x^2y$	$\frac{1}{24}$	∞	∞
Pullen-Edmonds [15]	$\frac{1}{2}(x^2+y^2)+ax^2y^2$			
	$a=-0.5$	0.5 +	$\simeq 0.32$	0.5 +
	$a>0$	$\frac{3}{4a}-$	$\frac{3}{4a}-$	$\simeq\frac{0.42}{a}$

to show that periodic orbits, if they exist in certain regions of configuration space of these Hamiltonian, are isolated and unstable. This function may be argued [13] to be the projection of the velocity of geodesic separation onto x, y space. We may also construct this by making mathematical the question: when two trajectories cross a contour line, are they forced apart by the shape of the contour, or squeezed together?

Consider at a point (x, y) a vector ϱ along the force $(-V_x, -V_y)$. A minimal energy trajectory would be along ϱ. The normal to ϱ, say ζ would then be $(V_y, -V_x)$, and the velocity of deviation would then be

$$\begin{aligned}\zeta\cdot((\nabla_\zeta)\varrho) &= \chi(x,y)\\ &= V_{xx}V_y^2+V_{yy}V_x^2-2V_xV_yV_{xy}\,. \quad (6)\end{aligned}$$

With this we may then reformulate the conclusion from the Jacobi equation, or the TBD criterion as: *the system will look stochastic if the rate of change of χ along the force is positive.*

We summarize the results (indicated as E_c(PS)) of this rather straightforward application in Table 1, along with a comparison with the exact (numerical) and TBD predicted values for the critical energy. Not all the successes of our criterion nor all the failures of the TBD criterion are cited. For the masses not equal to unity (6) has a simple modification [13].

Note that for the Pullen-Edmonds potential the energy they cite themselves is for when a "significant fraction" of the trajectories display stochasticity. In the same vein, we cite the lowest well-documented value in each case; for the Barbanis potential for example, Fig. 1 in [16] shows the area (of the poincare plane) that shows stochasticity to be non-zero at $E>0.005$, which is the figure we cite*.

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* *Note added in proof:* In the five years since this talk was presented, substantial work has been done on this issue by Pettini and co-workers. See, for example, M. Cerruti-Sola and M. Pettini, Phys. Rev. E, **53,** 179 (1996).

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