

## NORMALIZATION OF RESONANT HAMILTONIANS

David Farrelly,\* Jeffrey Humphreys,<sup>†</sup> and T. Uzer<sup>‡</sup>

\*Department of Chemistry and Biochemistry  
Utah State University, Logan, UT 84322-0300, U.S.A.

<sup>†</sup>Department of Mathematics and Statistics  
Utah State University, Logan, UT 84322-3000, U.S.A.

<sup>‡</sup>School of Physics, Georgia Institute of Technology,  
Atlanta, GA 30332-0430, U.S.A.

### INTRODUCTION

The definition of integrability is simple to state: an autonomous  $N$  degree of freedom Hamiltonian is integrable if  $N$  independent global invariants exist and these are in involution with each other.<sup>1</sup> However, a failure to find such a set of global invariants does not exclude the possibility that the Hamiltonian in question is integrable. The detection of integrability is thus a critical issue in non-linear dynamics and a variety of analytical and numerical procedures has been developed to determine if a Hamiltonian is integrable. The most obvious approach is to try to establish if the Hamiltonian is separable, possibly using the Stäckel conditions to guide one to appropriate coordinate system. It should be noted, however, that finding coordinates that separate a particular problem can itself be a difficult task. More general and systematic approaches than simply seeking separability are therefore in order, e.g., the Whittaker program. An alternative method is the Painlevé test<sup>2</sup> in which the analytic structure of the equations of motion in the complex time plane is examined. This approach has been used to uncover integrability but must be applied gingerly because it cannot be guaranteed to succeed in every case. Probably the simplest numerical method is to generate Poincaré surfaces of section and determine by eye whether or not the motion is integrable. Of course, no numerical method by itself can definitively determine integrability.

Deprit and co-workers<sup>3-7</sup> in their studies of normal forms, and particularly in an application to the Toda Lattice<sup>3</sup> have discovered what might constitute a new symptom of integrability in Hamiltonian systems. They note a correlation between the persistence of degeneracy in the normal form to high order and integrability of the pre-normalized Hamiltonian, and conjecture that this might be a symptom of integrability.<sup>6</sup> However, tests of this conjecture have ultimately uncovered integrable systems that are also separable. In a recent study of a problem in atomic physics we have encountered a Hamiltonian possessing a non-separable, integrable limit.<sup>7</sup> Surprisingly, in this case the conjecture of Deprit and Miller seems not to hold which

led us to question whether normalization might sense separability rather than integrability *per se*. After all, it is well known quantum mechanically that separability leads to degeneracies and degenerate equilibria are the symptom that the normal form is supposed to exhibit in the case of integrability. In this paper we examine normalization of, (i) a class of perturbed isotropic oscillators to high order which admit various integrable limits, and, (ii) the hydrogen atom in a generalized van der Waals (GVDW) potential. We conclude that under certain circumstances normalization can detect separability, but that it may also overlook integrable cases, whether separable or not.

#### NORMALIZATION OF ELLIPTIC OSCILLATORS

The normalization of perturbed elliptic oscillators has been studied thoroughly by Deprit and co-workers.<sup>3-7</sup> In fact, our exhibition problem is the same as Miller's,<sup>8</sup> i.e., a perturbed elliptic oscillator of the form  $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$  where

$$\mathcal{H}_0 = \frac{1}{2}(P_x^2 + P_y^2) + \frac{1}{2}(x^2 + y^2) \quad (1)$$

and

$$\mathcal{H}_1 = \epsilon(\alpha x^3 + \beta xy^2) \quad (2)$$

High order normalizations of (i.e., 1:1 resonant) elliptic oscillators perturbed by quartic and sextic polynomials have also been investigated recently: for these systems the integrable limits also turn out to be globally separable.<sup>4-8</sup> To start it is useful to consider the properties of the isotropic oscillator  $\mathcal{H}_0$ , in particular its integrals of motion. Including the energy there are four invariants

$$\begin{aligned} \pi_0 &= E_0/2 = \frac{1}{4}(P_x^2 + x^2) + \frac{1}{4}(P_y^2 + y^2) \\ \pi_1 &= D/2 = \frac{1}{4}(P_x^2 + x^2) - \frac{1}{4}(P_y^2 + y^2) \\ \pi_2 &= L/2 = \frac{1}{2}(yP_x - xP_y) \\ \pi_3 &= K/2 = \frac{1}{2}(P_x P_y + xy). \end{aligned} \quad (3)$$

The  $\{\pi_i, i = 1, 2, 3\}$  are called the *Hopf* variables and are related in a simple fashion to  $D, L, K$  which correspond to the more usual definitions of the invariants of the isotropic oscillator. The Hopf variables have the useful property of satisfying the same Poisson bracket relations as angular momentum, namely,

$$\{\pi_j, \pi_k\} = \epsilon_{jkl}\pi_l \quad (4)$$

where  $\epsilon_{jkl}$  is equal to 1 (-1) for even (odd) permutations of its subscripts and to 0 otherwise. Together with the relation

$$\pi_0^2 = \pi_1^2 + \pi_2^2 + \pi_3^2 \quad (5)$$

the  $\{\pi_i, i = 1, 2, 3\}$  generate the Lie algebra of the group  $SU(2)$ . Equation (5) is that of a sphere, sometimes nominated the Poincaré sphere, and on whose surface the phase flow of the reduced system can be portrayed.

Further geometrical insight can be obtained by recognizing that the Hopf variables may be transformed to action-angle variables  $J_x, J_y, \phi_x, \phi_y$  as follows,

$$\begin{aligned} x &= \sqrt{2J_x} \sin \phi_x, & y &= \sqrt{2J_y} \sin \phi_y \\ P_x &= \sqrt{2J_x} \cos \phi_x, & P_y &= \sqrt{2J_y} \cos \phi_y \end{aligned} \quad (6)$$

After a further transformation

$$\begin{aligned} J_1 &= \frac{(J_x + J_y)}{2}, & J_2 &= \frac{(J_x - J_y)}{2} \\ \phi_1 &= \phi_x + \phi_y, & \phi_2 &= \phi_x - \phi_y \end{aligned} \quad (7)$$

the  $\{\pi_i\}$  become,

$$\begin{aligned} \pi_0 &= J_1 \\ \pi_1 &= J_2 \end{aligned}$$

$$\begin{aligned} \pi_2 &= \sqrt{J_1^2 - J_2^2} \cos \phi_2 \\ \pi_3 &= \sqrt{J_1^2 - J_2^2} \sin \phi_2 \end{aligned} \quad (8)$$

which makes clear that the reduced phase space defined by  $\pi_0 = \text{constant}$  is a two-dimensional sphere. The action-angle variables just introduced are closely related to the coordinates of Hopf transformations between the Hopf variables may be effected by a simple rotation on the Poincaré sphere.

Our intuition, which springs from molecular spectroscopy, causes us to think of the unperturbed Hamiltonian  $\mathcal{H}_0$  as describing two modes (e.g., of a molecule) whose normal coordinates are taken to be  $x$  and  $y$ .<sup>8</sup> Working for now with the unperturbed Hamiltonian it is possible to characterize the invariant tori of the system in terms of the  $\pi$ 's or the quantities  $D, K, L$ . We label  $D$ -type dynamics *normal* mode,  $L$ -type dynamics *precessional* mode, and  $K$ -type dynamics *local* mode in analogy with the terminology used in molecular spectroscopy. In light of the Poisson bracket relations of eq. (4),  $\pi_0$  and any one of  $D, K$ , and  $L$  (or linear combinations) may be used to parameterize the invariant tori of  $\mathcal{H}_0$ . The degeneracy of the unperturbed system means that any of the various possible representations are acceptable. Under the influence of a perturbation, however, it becomes critical to select the correct parameterization of the unperturbed tori. This must be done in such a way that, as one causes the perturbation to diminish, eventually to zero, the KAM tori of  $\mathcal{H}$  transmit smoothly into the invariant tori of  $\mathcal{H}_0$ . In fact the three Hopf variables are associated with separability of the isotropic oscillator in Cartesian ( $\pi_1$ ), polar ( $\pi_2$ ), and rotated Cartesian coordinates ( $\pi_3$ ). Importantly, rotations in the phase space coordinates transform the Hopf variables into each other, as can be proven by explicit calculation or by  $SU(2)$  rotations on the Poincaré sphere.

Normalization of an elliptic oscillator perturbed by a real polynomial in the coordinates  $(x, y)$  about the center at the origin is guaranteed to produce an expansion in which each term is a polynomial in the  $\pi$ 's. In the event that this polynomial is a function of a single Hopf variable the implication is that the dynamics of the reduced system is of purely local, normal or precessional mode nature. Does this imply anything regarding separability or integrability? It is time to normalize the exhibition problem.