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Monodromy in perturbed Kepler systems: hydrogen atom in crossed fields

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Abstract. – We demonstrate that an integrable approximation to the hydrogen atom in orthogonal electric and magnetic fields has monodromy, a fundamental dynamical property that makes a global definition of action-angle variables and of quantum numbers impossible. When the field strengths are sufficiently small, we find our integrable approximation using a two step normalization procedure. One of dynamically invariant sets of the resulting integrable system is a doubly pinched torus whose existence proves the presence of monodromy.

Introduction. – In 1980 Duistermaat [1] introduced the concept of monodromy in the study of two degree of freedom integrable Hamiltonian systems. Since that time monodromy has been analyzed in several integrable systems of classical mechanics [2]. Monodromy describes the global twisting of a family of invariant 2-tori parameterized by a circle of regular values of the energy momentum map of the integrable system. Its presence is signaled by the existence of a singular fiber of the energy momentum map which is topologically a “pinched torus” [3]. Loosely speaking, if an integrable system has monodromy, then it is impossible to label the tori in a unique way by values of the actions. Since invariant tori are at the foundation of semiclassical EBK quantization of integrable systems, monodromy should manifest itself in the corresponding quantum systems [4, 5, 6]. Because monodromy is quite common in classical integrable systems of two degrees of freedom, it should have many important physical implications in quantum mechanics.

In this note we report the results of the analysis of the geometry of an integrable approximation to the problem of the hydrogen atom in crossed magnetic and electric fields. (This fundamental physical system is an atomic analog [7] of a perturbed Keplerian system.) We show that its geometry is nontrivial and has monodromy.

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Our work is largely based on the original study in [8] (see the discussion in [2, 9]) and the recent first normal form analysis in [10]. We should mention the work on atom in fields problems with axial symmetry [11, 12] which implicitly uses the idea of the second reduced phase space, as well as [13, 14] where the concept of a dynamical S^1 symmetry (and its corresponding "third" integral) is visibly present.

The crossed fields problem. – The Hamilton function of the hydrogen atom in the presence of constant orthogonal magnetic and electric fields [7] is

$$H = \frac{\mathbf{P}^2}{2} - \frac{C}{|\mathbf{Q}|} + FQ_2 + \frac{1}{2}G(Q_2P_3 - Q_3P_2) + \frac{1}{8}G^2(Q_2^2 + Q_3^2). \qquad (1)$$

The direction of the magnetic and electric fields are, respectively, 1 and 2; Q's are the coordinates in the physical 3-space, $\mathbf{P}$ is the 3-vector of conjugate momenta [15]. The first two terms in the right hand side of (1) represent the Kepler Hamiltonian, the third is the electrostatic potential describing Stark effect, and the two last terms describe linear and quadratic Zeeman effect. We have introduced an "effective charge" C in order to have the same kind of parameters as in equation (1.1) of [8]. This latter equation is equivalent to (1) with the quadratic Zeeman term omitted and thus can be interpreted as a case when the magnetic field strength G is small.

A priori the Hamiltonian (1) has a finite symmetry group of order 4, which is isomorphic to $\mathbf{Z}_2 \times \mathbf{Z}_2$ [10]. Its three nontrivial elements are C_s, which is the spatial reflection in the plane orthogonal to axis G, and the operations T_2 and T_s given by the composition of the anti-symplectic momentum reversal $P \to -P$ (also called time reversal) and a rotation by π around the axis F and a reflection in the plane (GF), respectively. We will see that properly taking these finite symmetries in account considerably simplifies the analysis.

First normal form. – To determine whether our Hamiltonian system has monodromy, we regularize the Hamiltonian (1) using Kustaanheimo-Stiefel (KS) method, normalize it *twice* and study the resulting integrable system. After the first normalization we truncate at order 2 and obtain the first normal form $\mathcal{H}_{\mathrm{nf}}$, which has the regularized Kepler Hamiltonian $2N$ (=oscillator Hamiltonian) as an integral of motion. (For our original Hamiltonian system $2N$ is an approximate integral of motion). We give some more details on finding $\mathcal{H}_{\mathrm{nf}}$.

The KS normalization of the perturbed Kepler Hamiltonian has been implemented in the atom-in-fields problem by several authors. We follow the recent computation in [10] where a particularly efficient field parameterization is introduced. We scale the dynamical variables in the Hamiltonian (1) so that the effective charge in the Coulomb potential becomes 1. Then we regularize by rescaling time $dt \to dt/4r$ and apply the KS map $M_{\mathrm{KS}} : \mathbf{R}^8 \to \mathbf{R}^6 : (q,p) \to (Q,P)$. In KS variables our Hamiltonian becomes a perturbed 1:1:1:1 resonant oscillator $2N = \frac{1}{2}(p^2 + q^2)$ with frequency $\omega = \sqrt{-8E}/C$. We scale time again, so that the frequency of this oscillator becomes 1. The resulting KS Hamiltonian is

$$\frac{4}{\omega} = H = \frac{1}{2}(p^2+q^2) + \frac{1}{3}f(q_1q_2 - q_3q_4)^2q^2 + \frac{1}{2}g(q_2p_3 - q_3p_2)q^2 + \frac{1}{8}g^2(q_1^2+q_4^2)(q_2^2+q_3^2)q^2,$$

where the field parameters

$$g = \varepsilon\alpha = G\left(\frac{2}{\omega C}\right)^2, \quad f = \varepsilon\beta = 3F\left(\frac{2}{\omega C}\right)^3, \qquad (2)$$

have been scaled so that their powers correspond to the degree in (q,p) of the corresponding perturbation terms. The uniform smallness parameter ε keeps track of the orders in the normal form [15]. An important feature of this parameterization is that we can describe *all* possible relative configurations of the two fields from the pure Stark ($G=0$) to the pure Zeeman ($F=0$) limit using the dimensionless quantities

$$\alpha \geq 0, \quad \beta \geq 0, \quad \alpha^2+\beta^2=1, \tag{3}$$

and the scaled uniform field intensity $2\varepsilon/\omega$. Our α and β give a nice S^1 parameterization of the first order Stark-Zeeman perturbation term, whose advantages become clear when computing the second normal form.

The KS Hamiltonian H is normalized in [10] using the usual Lie series method [16]. Truncating the result at second order gives the first normal form $\mathcal{H}_{\rm nf}$ (see eqs. (43) and (44) of [10]). Using a polynomial integrity basis (which is more efficient than just a Gröbner basis), we express the terms in $\mathcal{H}_{\rm nf}$ as polynomials in the oscillator invariants K_1, K_2, K_3 and L_1, L_2, L_3 (which are the components of Keplerian modified eccentricity [17] and angular momentum vectors, respectively, in KS variables). After reducing the oscillator and KS symmetry of the first normal form on the $2n$-level set of the oscillator Hamiltonian $2N$, we obtain the first reduced Hamiltonian

$$\mathcal{H}_n = \mathcal{H}_1 + \frac{\varepsilon}{2}\mathcal{H}_2 = (\alpha L_1 + \beta K_2) + \frac{\varepsilon}{2}\mathcal{H}_2, \tag{4}$$

where

$$\mathcal{H}_2 = \frac{\beta^2}{12}(3L_2^2 - 17K_2^2) + \frac{\alpha\beta}{3}(7K_2L_1 - L_2K_1) - \frac{\alpha^2}{2}\left[\frac{3}{2}(L_1^2+K_1^2) + L_2^2 + L_3^2 - K_2^2 - K_3^2\right],$$

and the constant terms are dropped. Note that on the $2n$-level set of $2N$ our invariants satisfy the relations

$$K_1^2+K_2^2+K_3^2+L_1^2+L_2^2+L_3^2 = n^2 \quad \text{and} \qquad K_1L_1+K_2L_2+K_3L_3=0, \tag{5}$$

and have Poisson brackets generating so(4). The Casimirs in (5) define the first reduced phase space $S_n^2 \times S_n^2$, the product of two 2-spheres of radius n. Thus removing the Keplerian and KS symmetry from the first normal form gives a two degree of freedom system on $S_n^2 \times S_n^2$ with Hamiltonian $\mathcal{H}_n$.

Second normal form. – The second normalization introduced in [8] has not been used before in perturbed hydrogen atom studies. To perform this normalization we look at the first order term $\mathcal{H}_1$ in $\mathcal{H}_n$ (4). The Hamiltonian vector field $X_{\mathcal{H}_1}$ has a flow which generates an S^1 symmetry on $S_n^2 \times S_n^2$. This is an approximate dynamical symmetry of the first normal form. Averaging $\mathcal{H}_n$ with respect to the flow of $X_{\mathcal{H}_1}$ gives the second normal form $\mathcal{H}_{\rm snf}$. Note that $\mathcal{H}_1$ is an integral of the Hamiltonian system corresponding to $\mathcal{H}_{\rm snf}$. We give some more details on how to obtain $\mathcal{H}_{\rm snf}$. To represent the flow of $X_{\mathcal{H}_1}$ we take advantage of our parameterization (α,β) and define an automorphism of the Poisson algebra

$$(K,L) \to (T,V) = (\alpha L_1 + \beta K_2, \alpha L_2 - \beta K_1, L_3, \beta L_2 + \alpha K_1, \alpha K_2 - \beta L_1, K_3),$$

which is a rotation. This transformation naturally preserves the Casimirs in (5) and also the so(4) Poisson bracket relations. It can be seen that after dropping the constant terms and rescaling time yet again, the first reduced Hamiltonian becomes $\mathcal{H}_{\rm n} = T_1 + \frac{1}{2}\varepsilon\mathcal{H}_2$ and that $\mathcal{H}_1 = T_1$ generates a dynamical symmetry group S^1. To find the second normal form it suffices to average $\mathcal{H}_2$ over the integral curves of the Hamiltonian vector field X_{T_1}. We express the resulting second normal form $\mathcal{H}_{\rm snf} = T_1 + \frac{1}{2}\varepsilon\overline{\mathcal{H}}_2$ as a function of the invariants of the flow of X_{T_1}. The algebra of all polynomial invariants of this flow is generated by the functions

$$N^2 = T^2+V^2, \quad T_1, \quad \pi_1 = V_1, \quad \pi_2 = T_2^2+T_3^2-V_2^2-V_3^2, \quad \pi_3 = 2(T_2V_3 - T_3V_2). \tag{6}$$

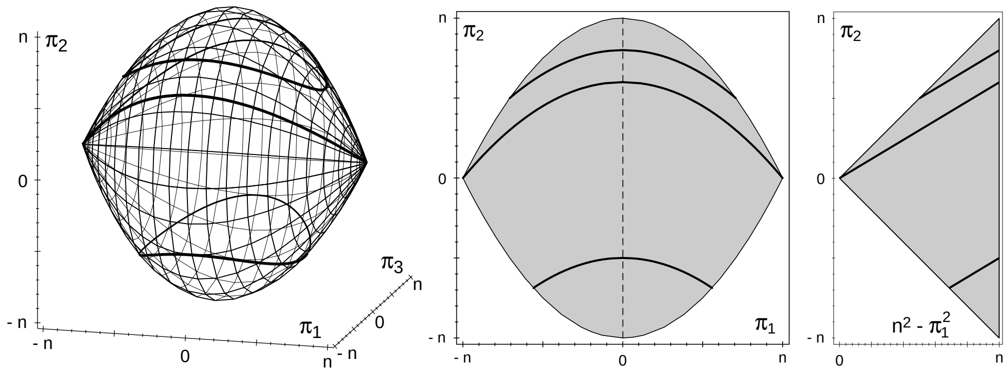

Fig. 1. – Singular reduced phase space $P_{n,0}$ (left), its projection on the $\pi_3 = 0$ plane (center), fully symmetry reduced space $W_{n,0}$ (right). Level sets correspond to the case with monodromy, $a/b = -0.6$.

The last three functions are algebraically dependent and satisfy the relation

$$\pi_3^2 + \pi_2^2 = \left[n^2 - (c+\pi_1)^2\right]\left[n^2 - (c-\pi_1)^2\right]. \tag{7}$$

Here the values of N and T_1 are fixed at n and c respectively. The above relation is obtained directly using (5) and is the only relation among the invariants π_1, π_2 and π_3. Furthermore, functions π_1 and π_3 are covariants of the $\mathbf{Z}_2 \times \mathbf{Z}_2$ action, which is naturally preserved by the flow of X_{T_1}. It follows that the *only* invariants necessary to express $\mathcal{H}_{\rm snf}$ are the integrals N, T_1, and the functions π_1^2 and π_2 which satisfy no auxiliary relations. We fix the values of N and T_1, drop the additive constant, and arrive at the second reduced Hamiltonian

$$\mathcal{H}_{n,c} = n\frac{\epsilon}{8}\left[2\alpha^2\pi_2 + (1-4\alpha^2-2\alpha^4)(n^2-\pi_1^2)\right] = a\pi_2 + b(n^2-\pi_1^2) = h. \tag{8}$$

Singular second reduced phase space. – The Hamiltonian $\mathcal{H}_{n,c}$ is defined on the second reduced phase space $P_{n,c}$. Because the S^1 action defined by X_{T_1} on

$$M_c = \mathcal{H}_1^{-1}(c) \cap (S_n^2 \times S_n^2) \tag{9}$$

has fixed points, we must use *singular reduction* [2] to obtain a parameterized family of second reduced phase spaces $P_{n,c}$. The geometry of $P_{n,c}$ can be easily analyzed in terms of the invariants of the flow of X_{T_1}. This has been treated at length in [8, 9, 2, 18]. We give some more details. Equation (7) suggests that the second reduced phase space $P_{n,c}$ can be realized as a semi-algebraic variety in $\mathbf{R}^3$. Indeed, $P_{n,c}$ is a surface of revolution defined by (7) together with the inequalities

$$|c| \le n, \quad |\pi_1| \le n - |c|, \quad |\pi_2| \le n^2 - c^2, \quad |\pi_3| \le n^2, \tag{10}$$

which specify the domain of definition of (5), (6) and (7). From this explicit description we see that $P_{n,c}$ is a sphere in $\mathbf{R}^3$ when $|c| < n$. If $0 < |c| < n$ this sphere is smooth, but if $c = 0$ it has two conical points at $(\pi_1, \pi_2) = (\pm n, 0)$, that is, $P_{n,0}$ is *singular* (fig. 1, left). Note that in a number of papers on this and similar systems [11, 13] authors represent their problem as a rotator. In other words, they map $P_{n,c}$ to a sphere. When $c = 0$ this map is, of course, singular. Hiding this singularity has hindered their analysis. In fact, the space $P_{n,0}$ is of primary interest to us. Its two singular points form an orbit of a $\mathbf{Z}_2$ subgroup of $\mathbf{Z}_2 \times \mathbf{Z}_2$ and thus have the same value of $\mathcal{H}_{n,0}$ (8), namely, $h = 0$.

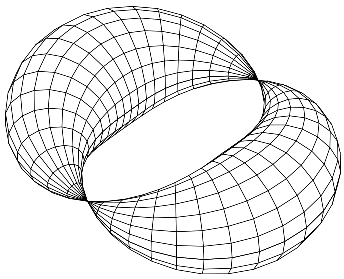

Fig. 2. – Doubly pinched torus: a heteroclinic connection of stable and unstable manifolds.

We have already used the finite symmetry $\mathbf{Z}_2 \times \mathbf{Z}_2$ of our problem (1) to express the second reduced Hamiltonian $\mathcal{H}_{n,c}$ most compactly. Arguing along the same lines, we can reduce the action of $\mathbf{Z}_2 \times \mathbf{Z}_2$ on $P_{n,c}$ itself. This reduction is illustrated in fig. 1, where we first reduce the $\mathbf{Z}_2 : \pi_3 \to -\pi_3$ symmetry to get a planar section of $P_{n,0}$ (fig. 1, center) and then reduce again with respect to $\mathbf{Z}_2$ symmetry $\pi_1 \to -\pi_1$ to obtain the *fully symmetry reduced space* $W_{n,0}$ (fig. 1, right). The coordinates on $W_{n,0}$ are (π_1^2, π_2), which are exactly the invariants of the $\mathbf{Z}_2 \times \mathbf{Z}_2$ action used to express the second reduced Hamiltonian $\mathcal{H}_{n,c}$ (8).

Qualitative analysis of the singular second reduced problem. – We now consider the geometry of the constant level sets of the second reduced Hamiltonian $\mathcal{H}_{n,0}$ on the singular second reduced phase space $P_{n,0}$ and lift them back to the space M_0 in (9). In other words, we look at the level sets of the energy momentum mapping of the integrable system $(\mathcal{H}_{\rm snf}, \mathcal{H}_1)$

$$\mathcal{EM} : S_n^2 \times S_n^2 \to \mathbf{R}^2 : p \to (\mathcal{H}_{\rm snf}(p), \mathcal{H}_1(p)) \tag{11}$$

and show that for an open interval $\mathcal{I}$ of field parameter α, the $(h, c) = (0, 0)$-level set $\mathcal{EM}^{-1}(0, 0)$ (that is, the set of all points in $S_n^2 \times S_n^2$ where $\mathcal{H}_1$ and $\mathcal{H}_{\rm snf}$ both take the value zero), is a doubly pinched 2-torus in $S_n^2 \times S_n^2$. Hence the energy momentum map $\mathcal{EM}$ has monodromy.

We start with the fully symmetry reduced space $W_{n,0}$ where the h-level sets of $\mathcal{H}_{n,0}$ in (8) are represented by *straight lines* [19]. Our task here is particularly simple and we focus on the situation when $|b/a| < 1$, that is, when

$$\alpha^2 \in \mathcal{I} = \left(\frac{\sqrt{6}}{2} - 1, \frac{\sqrt{2}}{2} \right). \tag{12}$$

In this case the 0-level set of the second reduced Hamiltonian $\mathcal{H}_{n,0}$ has special topology: it is a union of an interval and a singular point. We lift the level sets of $\mathcal{H}_{n,0}$ from $W_{n,0}$ to $P_{n,0}$ as illustrated in fig. 1, right to left. Next we reconstruct the 0-level set of $\mathcal{H}_{n,0}$ on M_0, that is we find the corresponding dynamically invariant set of the first reduced Hamiltonian $\mathcal{H}_n$. To do this we make use of the reduction map

$$\Pi : M_0 \subseteq S_n^2 \times S_n^2 \to P_{n,0} \subseteq \mathbf{R}^3 : (T, V) \to \Big(\pi_1, \pi_2(T, V), \pi_3(T, V)\Big).$$

The fiber $\Pi^{-1}(p)$ of the map Π over the point $p \in P_{n,0}$ is a unique orbit of X_{T_1} on M_0. If p is a nonsingular point, then $\Pi^{-1}(p)$ is a circular orbit S^1, otherwise it is an equilibrium point [specifically, $(V, T) = \pm(0, 0, 0, 1, 0, -1)$]. If we now look at the 0-level set of $\mathcal{H}_{n,0}$ on $P_{n,0}$ (fig. 1, left), which is a circle with two singular points p_1 and p_2, we realize that after reconstruction the points p_1 and p_2 remain points on $S_n^2 \times S_n^2$ while any other point of this

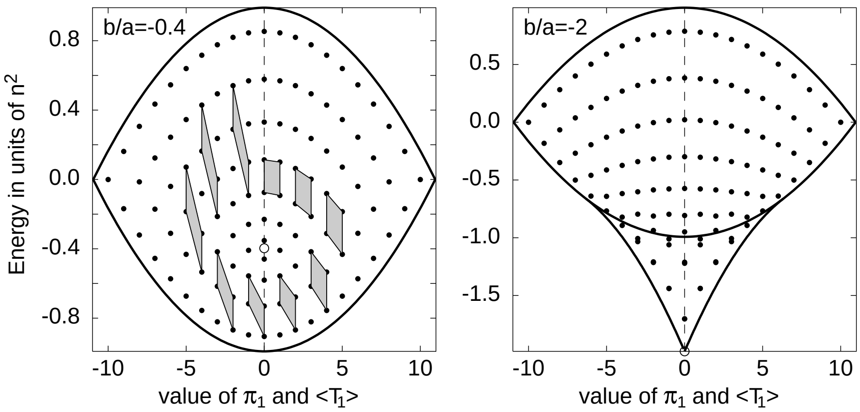

Fig. 3. – Quantum and classical energy momentum map for quantum number $n = 11$ and classical value $n_{\rm cl} = \sqrt{120}$. In the case with monodromy (left) the position of the pinched torus is marked by a white circle and the deformation of the local lattice is shown by a sequence of shaded quadrilaterals.

circle becomes an S^1. Thus reconstruction of the 0-level set of the second reduced Hamiltonian gives a doubly pinched 2-torus (fig. 2) in M_0 [18]. Using the results of [3] we conclude that the energy momentum map (11) has monodromy when α^2 lies in the interval $\mathcal{I}$.

Quantum monodromy. – Monodromy is well manifested in quantum mechanics where regular sequences of invariant tori are selected by the EBK quantization conditions [4, 5]. Locally these tori and the corresponding quantum levels can be labeled by the values of (quantized) actions but any global labeling is impossible if monodromy is present.

We construct the quantum analog of the Hamiltonian (8) in terms of the $su(2) \times su(2)$ algebra of quantum operators $\mathbf{T} \pm \mathbf{V}$ and solve a simple matrix problem at a fixed value of quantum number $n = \langle \mathbf{T}^2 + \mathbf{V}^2 \rangle = 1, 2, \ldots$, for all values of quantum number $m = \langle T_1 \rangle = -(n-1), \ldots, n-1$. (Note that the classical value of the Kepler integral N is $\sqrt{n^2 - 1}$.) This calculation essentially reproduces [20]. Resulting quantum energies are shown by dots in fig. 3. Bold lines in this figure represent stationary points of $\mathcal{H}_{n,0}$ on $P_{n,0}$. They limit the range of the classical energy momentum map $\mathcal{EM}$. Quantum energies form a 2-lattice in the range of $\mathcal{EM}$. In the presence of monodromy this lattice has a *point defect* located at the value of $\mathcal{EM}$ corresponding to the pinched torus. The type of the defect is related to the number of pinched points. If we now define an elementary cell of the lattice and take it along a path which lies entirely in the domain of regular values of $\mathcal{EM}$ and goes around the defect (see, fig. 3, left), we can easily follow the evolution of this cell because each small step to a neighbor cell is unambiguous. However, after making a tour our cell does *not* match the original cell! [The accumulated deformation is described by the matrix $\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}$ where 2 corresponds to the number of pinched points.] Thus the lattice cannot be labeled globally by two quantum numbers.

For comparison, we show the results of the same calculation for α^2 outside the monodromy interval $\mathcal{I}$ (fig. 3, right). This case is well known in the quadratic Zeeman effect [21]. Two distinct regions in the range of $\mathcal{EM}$ are clearly separated by the energy of a $\mathbf{Z_2}$ symmetric stationary point of $\mathcal{H}_{n,c}$. In the upper region the quantum lattice corresponds to that of a rotator with quantum number $j = n, n-1, \ldots$. The lower region corresponds to the double well 2-oscillator. Over each of the regions labeling is straightforward.

Discussion. – Our present work raises several interesting questions. We have relied on normalization to find an integrable approximation to an essentially non-integrable system. Most of the invariant tori of the integrable system survive to KAM tori. Since these KAM tori fit together into smooth families of tori, the monodromy present in the integrable approximation survives perturbation and as such exists in the hydrogen atom problem in orthogonal electric and magnetic fields when the parameter α lies in the interval $\mathcal{I}$. Similar questions are associated with "quantum monodromy". We are convinced that for a sufficiently small perturbation the quantum energy level structure of our system is similar to the one analyzed in this paper.

The perturbed hydrogen atom in crossed fields continues to attract considerable interest of experimentalists [22]. Application of the idea of monodromy to experimental studies depends on how the questions discussed above are answered. We think that our system will be important in experimental studies because one can tune the parameter α so that it goes in and out of the region where monodromy occurs.

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