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Perturbations of the hydrogen atom by inhomogeneous static electric and magnetic fields

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Abstract. The hydrogen atom is a specific, and physically relevant, Keplerian 2-body system with one of the bodies assumed infinitely heavy. Isochronous integrable n -shell approximations for the perturbations of the hydrogen atom, known as Stark and Zeeman effects in the presence of homogeneous electric and magnetic fields, respectively, have been widely studied. In order to go beyond the set of linear systems, we considered perturbations by inhomogeneous electromagnetic fields. In particular, we found that the perturbation by a generic inhomogeneous magnetic field results in an approximately integrable anisochronous system which can be described as two rigid Euler tops coupled through higher order terms.

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1. Introduction

The hydrogen atom is the quantum analogue of a specific Keplerian two-body system where one of the bodies is assumed infinitely heavy[‡] and resting at the origin. The obvious classical analogues of this system can be found in the motion around a star of an artificial satellite or of a planet. The unperturbed system is described (in atomic units) by the Hamiltonian

$$H_0 = \frac{\|\mathbf{P}\|^2}{2} - \frac{1}{\|\mathbf{Q}\|}, \quad (1)$$

where \mathbf{Q} are position coordinates in the physical space \mathbb{R}^3 , and \mathbf{P} are the corresponding canonically conjugate momenta. Perturbations of this system by external electric and magnetic fields, known respectively as Stark and Zeeman effect, are among the most widely studied systems since the beginnings of quantum mechanics and modern atomic physics in 1930’s and the subject of many publications and monographs. We refer to the recent review paper [1] for further bibliography and most technical details.

[‡] The proton mass m_p is about 1836 times the mass of the electron m_e which equals 1 atomic unit.

In the case of sufficiently weak fields, the system can be considered as a small perturbation of (1) and an averaging procedure with respect to the Keplerian flow can be performed. In quantum mechanics, this provides the so-called n -shell approximation, where the principal quantum number $n = 0, 1, 2, \dots$ corresponds to the classical Keplerian integral of motion. The corresponding classical reduced system is an Euler-Poisson system with compact phase space $\mathbb{S}^2 \times \mathbb{S}^2$. The reduced normalized (quantum and classical) Hamiltonian,

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 + \dots \quad (2)$$

can be written as function of the Keplerian invariant n , the angular (orbital) momentum vector $\mathbf{L} = \mathbf{Q} \times \mathbf{P}$ and the scaled eccentricity vector \mathbf{K} . These are subject to two constraints:

$$\|\mathbf{L}\|^2 + \|\mathbf{K}\|^2 = n^2 \quad \text{and} \quad \mathbf{L} \cdot \mathbf{K} = 0. \quad (3)$$

Alternatively, we can use two angular momentum vectors of equal length

$$\mathbf{J}_1 = \frac{\mathbf{L} + \mathbf{K}}{2} \quad \text{and} \quad \mathbf{J}_2 = \frac{\mathbf{L} - \mathbf{K}}{2},$$

for which the relations (3) become

$$\|\mathbf{J}_1\| = \|\mathbf{J}_2\| = \frac{n}{2}. \quad (4)$$

So $\mathbb{S}^2 \times \mathbb{S}^2$ can be realized in the ambient space \mathbb{R}^6 with coordinates $(\mathbf{J}_1, \mathbf{J}_2)$. The normal form (2) is a formal series in (\mathbf{L}, \mathbf{K}) (or \mathbf{J}_1 and \mathbf{J}_2). Its zero order, the normal form of the Keplerian Hamiltonian (1),

$$\mathcal{H}_0 = 2n$$

is a constant (on $\mathbb{S}^2 \times \mathbb{S}^2$), while each higher order term \mathcal{H}_k equals n times a homogeneous polynomial in (\mathbf{L}, \mathbf{K}) of degree k .

The classical system on $\mathbb{S}^2 \times \mathbb{S}^2$ is equipped with the Poisson algebra $\mathfrak{so}(4) \cong \mathfrak{so}(3) \oplus \mathfrak{so}(3)$, where each factor is generated by the components of the respective angular momentum \mathbf{J}_1 or \mathbf{J}_2 in a standard way. The corresponding quantum system with Hamiltonian $\mathcal{H}(\hat{\mathbf{J}}_1, \hat{\mathbf{J}}_2)$ can be solved in the eigenbasis

$$|j_1, m_1\rangle |j_2, m_2\rangle \quad \text{with} \quad j_1 = j_2 = j \quad \text{and} \quad m_i = -j, -j+1, \dots, j-1, j$$

of the angular momentum operators $\hat{\mathbf{J}}_i^2$ and $\hat{\mathbf{J}}_{i,1}$. Note that in the quantum context, we should distinguish the quantum number j , the shell quantum number n , and the length

$$\|\hat{\mathbf{J}}_i\| = \langle j, m | \hat{\mathbf{J}}_i^2 | j, m \rangle^{1/2} = \sqrt{j(j+1)} \approx j + \frac{1}{2} \quad \text{for} \quad j \gg 1.$$

Similarly, in the semiclassical limit of large j , the classical Keplerian action N equals $2j+1 = n+1$. To avoid baroque notation, we will not distinguish between classical and corresponding quantum quantities unless both appear together in the same context.

1.1. Stark-Zeeman effect in spatially homogeneous fields

The most widely studied case of the Stark-Zeeman effect (see [1]) is the perturbation by static spatially homogeneous fields with Hamiltonian

$$H(\mathbf{Q}, \mathbf{P}) = H_0(\mathbf{Q}, \mathbf{P}) + \mathbf{F} \cdot \mathbf{Q} + \frac{1}{2} \mathbf{G} \cdot \mathbf{L} + \frac{1}{8} \|\mathbf{G} \times \mathbf{Q}\|^2. \quad (5)$$

After the Keplerian normalization and reduction of (5), we obtain in the first and principal order (because \mathcal{H}_0 becomes a constant)

$$\mathcal{H}_1(\mathbf{L}, \mathbf{K}) = n(\mathbf{g} \cdot \mathbf{L} + \mathbf{f} \cdot \mathbf{K}) = n(\mathbf{a}_1 \cdot \mathbf{J}_1 + \mathbf{a}_2 \cdot \mathbf{J}_2).$$

where the constant vectors \mathbf{f} and \mathbf{g} are scaled field parameters \mathbf{F} and \mathbf{G} and $\mathbf{a}_1 = \mathbf{g} + \mathbf{f}$, $\mathbf{a}_2 = \mathbf{g} - \mathbf{f}$. Since the flow $\varphi_{\mathcal{H}_1}^t$ of the Hamiltonian \mathcal{H}_1 is linear on $\mathbb{S}^2 \times \mathbb{S}^2$, and thus integrable, the Keplerian normal form (2) can be averaged again. This *second normalization* [1] with regard to $\varphi_{\mathcal{H}_1}^t$ gives an integrable system on $\mathbb{S}^2 \times \mathbb{S}^2$ do not vary significantly from torus to torus.

Two kinds of second normalization are possible. First rotating $\mathbf{J}_i \mapsto A_i \mathbf{J}_i = \tilde{\mathbf{J}}_i$ on each sphere $i = 1, 2$ in $\mathbb{S}^2 \times \mathbb{S}^2$ and with $A_i \in \text{SO}(3)$, we can transform \mathcal{H}_1 into

$$\mathcal{H}_1(\mathbf{L}, \mathbf{K}) = \omega_1 \tilde{J}_{11} + \omega_2 \tilde{J}_{21}.$$

where $\omega_i = n \|\mathbf{a}_i\|$. If the frequencies ω_i are strongly non-resonant, we can reduce the regular \mathbb{T}^2 flow $X_{\mathcal{H}_1}$ completely. In this case, \tilde{J}_{11} and \tilde{J}_{21} are two globally defined actions with values $\tilde{j}_{1,1}$ and $\tilde{j}_{2,1}$. The geometry of such system is trivial: all its regular tori $\mathbb{T}^2 \subset \mathbb{S}^2 \times \mathbb{S}^2$ are the fibres over points $\{(\tilde{j}_{1,1}, \tilde{j}_{2,1}), 2|\tilde{j}_{i,1}| < n\}$ inside the interior of the action space, while the corners and the points on the edges of the square represent fixed points and periodic orbits, respectively. This system is also almost isochronous.

Resonances of $\omega_{1,2}$ may further complicate the situation, and at the same time—make it interesting. Their quantum manifestation was first recognized in [2]. For resonant frequencies ω_1 and ω_2 only one global action (a momentum) μ can be defined, and the reduction of the corresponding \mathbb{S}^1 action brings us onto a two-dimensional compact phase space which is homeomorphic to \mathbb{S}^2 and singular for some specific values of μ [1, 3–5]. The system on $\mathbb{S}^2 \times \mathbb{S}^2$ with Hamiltonian \mathcal{H} remains (approximately) integrable, but can have critical fibres other than fixed points and periodic orbits, notably a bitorus, a curled torus, and a pinched torus. The presence of either of the last two fibres results in Hamiltonian monodromy. Since \mathcal{H}_1 is linear, its flow is isochronous and, when the second normal form is considered, its frequencies are only slightly perturbed by the higher order terms.

A notable example of singular reduction can be given for the axially symmetric field configuration where $\mathbf{f} = (f, 0, 0)^T$, $\mathbf{g} = (g, 0, 0)^T$ (parallel fields) and

$$\mathcal{H}_1(\mathbf{L}, \mathbf{K}) = n(fK_1 + gL_1) = n(g + f)J_{11} + n(g - f)J_{21}.$$

In this case, \mathcal{H} is already integrable, since it commutes with $J_{11} + J_{21}$, and it is natural to perform a reduction procedure with respect to the corresponding \mathbb{S}_1 action. The corresponding momentum L_1 , the first component of the orbital angular momentum \mathbf{L} , is a global action with values $m \in [-n, n]$. The reduced phase spaces P_m are diffeomorphic to \mathbb{S}^2 for all $0 < |m| < n$, while $P_{\pm n}$ are points and P_0 is a sphere with two singular points, similar to the one Richard Cushman called a “lemon” [6].

1.2. Beyond the most studied cases. The idea of this paper

In this paper we investigate what kind of perturbed Keplerian systems can be obtained as perturbations of the hydrogen atom by external fields other than those described in sec. 1.1.

One possibility would be to consider oscillating electromagnetic fields. In the simplest cases, for example when a circularly polarized field plus a static one

perpendicular to the polarization plane is present (see for instance [7]), it is possible to completely remove the time dependence by considering a rotating frame of reference. This, however, adds a centripetal term which is linear in the angular momentum components and cannot be removed. If the time dependence cannot be removed by simple means, for example this happens if we add a generic static field to a circularly polarized one, we have to consider an extended phase space (where an additional degree of freedom is added and time become a canonical coordinate) on which the dynamics is described by an (extended) time-independent Hamiltonian (sometimes called the Floquet Hamiltonian). In this case it is possible to employ standard perturbation theory to perform an average over the time coordinate (which is akin to an angle). When we consider Keplerian orbits whose frequencies are resonant with the frequency of the external field (this case is analysed for instance in [8]) it is not possible to remove completely the time dependence, and the averaged system is still time-dependent. This requires a considerably more complicated analysis. Finally, for those n -shells whose Keplerian frequency is not in resonance with the periodic field, a complete average removes the extra degree of freedom. A first order analysis accounts for the effects produced by the averaged field which are similar to the ones described in this paper produced by a static field, while a theory taking into account higher orders might exhibit new terms. In conclusion, the study of periodic fields either gives no clear advantage or is substantially more complicated. So in this paper we will consider only time independent fields.

In order to preserve the approximate Keplerian symmetry and be able to descend on $\mathbb{S}^2 \times \mathbb{S}^2$ the fields should remain sufficiently weak (relative to the value of n). Furthermore if we consider static fields, in order to eliminate \mathcal{H}_1 as a principal order, the homogeneous field components defined by the linear scalar and vector potentials ϕ and \mathbf{A} should vanish (or at least they should be made insignificant).

Considering analytic potentials ϕ and \mathbf{A} at $\mathbf{Q} = 0$, the next, and yet unexplored, possibility is given by perturbations by inhomogeneous fields described by quadratic potentials. These perturbations contribute to \mathcal{H}_2 , which is a homogeneous quadratic polynomial in the components of \mathbf{J}_1 and \mathbf{J}_2 , and, of course, to higher terms in (2). Typically we will obtain on $\mathbb{S}^2 \times \mathbb{S}^2$ a completely non-integrable system. We can also obtain a nontrivial approximately integrable *anisochronous* system. In the former case, \mathcal{H}_2 does not Poisson commute with any other function of $(\mathbf{J}_1, \mathbf{J}_2)$. On the other hand, if the system with Hamiltonian \mathcal{H}_2 is integrable then the frequencies vary significantly between regular tori. Finally, in the presence of a Lie symmetry on $\mathbb{S}^2 \times \mathbb{S}^2$, such an \mathbb{S}^1 symmetry, we will obtain a system similar to the axially symmetric system already described in sec. 1.1.

As an example of an interesting approximately integrable system, consider a linear combination $\mathcal{H}_2 = c_1 J_{11}^2 + c_2 J_{21}^2$ or, more generally, a linear combination of two reduced Euler top Hamiltonians. The motion of the tops is coupled through the higher order terms in \mathcal{H} . In this work, we show that any perturbation due to a purely vector potential without linear terms (inhomogeneous magnetic field) results in such a system. On the other hand, we also find that a more complex integrable system on $\mathbb{S}^2 \times \mathbb{S}^2$ known as the Manakov top [9] cannot be realized as a perturbation of the hydrogen atom by constant external fields.

Why should such systems be of any particular interest to physics? One of the important reasons is that the compactness of $\mathbb{S}^2 \times \mathbb{S}^2$ and the straightforward quantization procedure make them attractive for “low-cost” studies of quantum–classical correspondence in the context of quantum manifestations of dynamical

chaos, or the Nekhoroshev stability in perturbed integrable systems, and other such phenomena which would remain otherwise inaccessible even to modern computers due to the exponentially long times during which the classical dynamics should be investigated.

2. Spatially inhomogeneous perturbations

A static electromagnetic field (in the absence of charge and currents) is characterized by two vectors \mathbf{F} (electric field) and \mathbf{G} (magnetic field) satisfying Maxwell equations:

$$\begin{aligned}\nabla \cdot \mathbf{F} &= 0 \\ \nabla \times \mathbf{F} &= \mathbf{0} \\ \nabla \cdot \mathbf{G} &= 0 \\ \nabla \times \mathbf{G} &= \mathbf{0}.\end{aligned}\tag{6}$$

Since the domain on which the field is considered is simply connected, it is possible to define a scalar potential ϕ and a vector potential \mathbf{A} such that

$$\begin{aligned}\mathbf{F} &= -\nabla\phi \\ \mathbf{G} &= \nabla \times \mathbf{A}.\end{aligned}$$

Using the potentials, the Hamiltonian for the hydrogen atom in the presence of a static external electromagnetic field (in atomic units) can be rewritten as

$$H = \frac{\|\mathbf{P}\|^2}{2} - \frac{1}{\|\mathbf{Q}\|} + \mathbf{P} \cdot \mathbf{A}(\mathbf{Q}) + \frac{1}{2}\|\mathbf{A}(\mathbf{Q})\|^2 - \phi(\mathbf{Q}).\tag{7}$$

The fields alone don't determine uniquely the potentials and it is necessary to fix the gauge. A convenient choice is given by the multipolar (also known as line, point or Poincaré) gauge, defined by the conditions:

$$\begin{aligned}\mathbf{A}(\mathbf{Q}) \cdot \mathbf{Q} &= 0 \\ \phi(\mathbf{0}) &= 0 \\ \mathbf{A}(\mathbf{0}) &= \mathbf{0}.\end{aligned}$$

In this way, an explicit expression for the potentials, in terms of the fields, is given by (see for instance [10]):

$$\begin{aligned}\mathbf{A}(\mathbf{Q}) &= -\mathbf{Q} \times \int_0^1 \mathbf{G}(\lambda\mathbf{Q})\lambda d\lambda \\ \phi(\mathbf{Q}) &= -\mathbf{Q} \cdot \int_0^1 \mathbf{F}(\lambda\mathbf{Q})d\lambda.\end{aligned}$$

From Maxwell equations (6) we have that

$$\begin{aligned}\Delta\mathbf{F} &= \mathbf{0} \\ \Delta\mathbf{G} &= \mathbf{0},\end{aligned}$$

and therefore \mathbf{F} and \mathbf{G} are harmonic vector functions. Using the analyticity of harmonic functions, we can rewrite them as $\mathbf{F} = \mathbf{F}_0 + \mathbf{F}_1 + \dots$ and $\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_1 + \dots$

where the components of \mathbf{F}_k and \mathbf{G}_k are k -homogeneous polynomials. Consequently we can write $\mathbf{A} = \mathbf{A}_0 + \mathbf{A}_1 + \dots$ and $\phi = \phi_0 + \phi_1 + \dots$ where ϕ_k and \mathbf{A}_k are potentials for \mathbf{F}_k and \mathbf{G}_k respectively. We have that

$$\begin{aligned}\mathbf{A}_k(\mathbf{Q}) &= \frac{1}{k+2} \mathbf{G}_k(\mathbf{Q}) \times \mathbf{Q} \\ \phi_k(\mathbf{Q}) &= -\frac{1}{k+1} \mathbf{F}_k(\mathbf{Q}) \cdot \mathbf{Q}\end{aligned}$$

In particular, if \mathbf{G} and \mathbf{F} are linear, we can introduce two 3×3 matrices \mathbf{F} and \mathbf{G} such that

$$\begin{aligned}\mathbf{F}(\mathbf{Q}) &= \mathbf{F} \mathbf{Q} \\ \mathbf{G}(\mathbf{Q}) &= \mathbf{G} \mathbf{Q}\end{aligned}$$

Maxwell equations (6) are, in this case, equivalent to:

$$\begin{aligned}\text{tr } \mathbf{F} &= 0, \\ \mathbf{F} - \mathbf{F}^T &= 0, \\ \text{tr } \mathbf{G} &= 0, \\ \mathbf{G} - \mathbf{G}^T &= 0,\end{aligned}$$

and Hamiltonian (7) becomes:

$$H = H_0 + \frac{\mathbf{Q} \cdot \mathbf{F} \mathbf{Q}}{2} + \frac{\mathbf{L} \cdot \mathbf{G} \mathbf{Q}}{3} + \frac{\|\mathbf{Q} \times \mathbf{G} \mathbf{Q}\|^2}{18}, \quad (8)$$

where H_0 is the unperturbed Kepler Hamiltonian.

3. Kustaanheimo-Stiefel regularization

The n -shell approximation is defined by considering the normal form of H obtained through an averaging procedure over the flow of H_0 . In order to perform this average one has to deal with the singularity at the origin. A way to do this is through the Kustaanheimo-Stiefel regularization (introduced in [11]). In this section we will give a brief description of the procedure. By doing so we can introduce explicitly the rescaled field matrices \mathbf{A} and \mathbf{B} which replace \mathbf{F} and \mathbf{G} and absorb the unimportant constants. Further details are common with the approach developed earlier, see [1].

The crucial point of the regularization process is to consider, starting from the original Hamiltonian H , a new Hamiltonian H_{KS} whose orbits, on a given energy surface, correspond, up to a reparametrization of time, to the ones of H . The flow is now complete and it is shown that H_{KS} , as a system, is equivalent to a perturbed four dimensional oscillator in the $1 : 1 : 1 : 1$ resonance.

Let (q, p) be coordinates on $T^*(\mathbb{R}^4 \setminus \{0\}) = \mathbb{R}^4 \setminus \{0\} \times \mathbb{R}^4$ and define the functions

$$\begin{aligned}Q(q) &= (Q_1(q), \dots, Q_4(q)) = (\mathbf{Q}(q), Q_4(q)) \\ P(q, p) &= (P_1(q, p), \dots, P_4(q, p)) = (\mathbf{P}(q, p), P_4(q, p))\end{aligned}$$

as:

$$\begin{aligned}Q(q, p) &= \mathbf{M}_{\text{KS}}(q)q \\ P(q, p) &= \frac{1}{2\|q\|^2} \mathbf{M}_{\text{KS}}(q)p\end{aligned}$$

where

$$M_{\text{KS}}(q) = \begin{pmatrix} q_1 & -q_2 & -q_3 & q_4 \\ q_2 & q_1 & -q_4 & -q_3 \\ q_3 & q_4 & q_1 & q_2 \\ q_4 & -q_3 & q_2 & -q_1 \end{pmatrix}$$

define also the function $\zeta(q, p)$ and the 1-form θ as

$$\begin{aligned} \zeta(q, p) &= -2\|q\|^2 P_4(q, p) = q_1 p_4 - q_4 p_1 + q_3 p_2 - q_2 p_3 \\ \theta &= q_4 dq_1 - q_1 dq_4 + q_2 dq_3 - q_3 dq_2. \end{aligned}$$

The functions $(\mathbf{Q}(q), \mathbf{P}(q, p))$ determine a surjective map Φ_{KS} from $T^*(\mathbb{R}^4 \setminus \{0\})$ onto $T^*(\mathbb{R}^3 \setminus \{0\})$. If H is a Hamiltonian on $T^*(\mathbb{R}^3 \setminus \{0\})$ it is possible to define its pullback H_{KS} on $T^*(\mathbb{R}^4 \setminus \{0\})$ as:

$$H_{\text{KS}}(q, p) = H(\mathbf{Q}(q), \mathbf{P}(q, p)).$$

The map Φ_{KS} itself is not symplectic, since it is straightforward to verify (using the fact that $\|q\|^{-1}M_{\text{KS}}(q)$ is orthogonal) that

$$\mathbf{P}(q, p) \cdot d\mathbf{Q}(q) = p \cdot dq + \|q\|^{-2}\zeta\theta.$$

However, it is immediate to see that ζ commutes with both \mathbf{Q} and \mathbf{P} (and hence with H_{KS}) and so, from Φ_{KS} , we can induce a function $\hat{\Phi}_{\text{KS}}$ obtained via symplectic reduction of $T^*(\mathbb{R}^4 \setminus \{0\})$ with respect to the \mathbb{S}^1 action of ζ on the hypersurface defined by $\zeta = 0$. $\hat{\Phi}_{\text{KS}}$ is a symplectic diffeomorphism. From a practical point of view it is sufficient to consider H_{KS} defined above as a Hamiltonian on $T^*(\mathbb{R}^4 \setminus \{0\})$ imposing the condition $\zeta = 0$ (this in general simplifies considerably the expressions involved).

If H is a Hamiltonian defined on $T^*(\mathbb{R}^3 \setminus \{0\})$ and $E \in \mathbb{R}$, we can consider the Hamiltonian:

$$\hat{H}(\mathbf{Q}, \mathbf{P}) = 4\|\mathbf{Q}\|(H(\mathbf{Q}, \mathbf{P}) - E) + 4.$$

Even though in general the flows of H and \hat{H} are not related, the energy surfaces $H^{-1}(E)$ and $\hat{H}^{-1}(4)$ coincide. On this common level set the orbits of H and \hat{H} are the same, up to a time reparametrization. If $H = H^{(0)} + V$ is the perturbed Kepler Hamiltonian, using the fact that (when $\zeta = 0$):

$$\begin{aligned} \|\mathbf{Q}(q)\| &= \|q\|^2 \\ \|\mathbf{P}(q, p)\|^2 &= \frac{\|p\|^2}{4\|q\|^2}, \end{aligned}$$

we have:

$$\hat{H}_{\text{KS}}(q, p) = \frac{\|p\|^2 + (-8E)\|q\|^2}{2} + \|q\|^2 V_{\text{KS}}(q, p)$$

where $V_{\text{KS}}(q, p) = V(\mathbf{Q}(q), \mathbf{P}(q, p))$. This shows that after regularization our system becomes a perturbed harmonic oscillator, in particular \hat{H}_{KS} can be defined in the origin and so we can consider $T^*\mathbb{R}^4$ as its natural phase space.

Defining $\Omega = \sqrt{-8E}$, we consider the canonical transformation:

$$(p, q) = (\Omega^{1/2}p', \Omega^{-1/2}q')$$

along with the time-energy rescaling:

$$(t, \hat{H}_{\text{KS}}) = (\Omega^{-1}t', \Omega\hat{H}'_{\text{KS}})$$

obtaining

$$\hat{H}'_{\text{KS}}(q', p') = 2n + v(q', p') = 4\Omega^{-1}$$

where

$$2n = \frac{\|q'\|^2 + \|p'\|^2}{2}$$

$$v(q', p') = \Omega^{-2}\|q'\|^2 F_{\text{KS}}(\Omega^{-1/2}q', \Omega^{1/2}p')$$

For the case of the hydrogen atom in an electromagnetic field defined by linear electric and magnetic fields $F(\mathbf{Q})$ and $G(\mathbf{Q})$, if

$$\begin{aligned} \mathbf{A} &= 8\Omega^{-4}\mathbf{F} \\ \mathbf{B} &= -3\Omega^{-3}\mathbf{G}, \end{aligned} \tag{9}$$

Hamiltonian (8) becomes:

$$H(q, p) = 2n + \frac{1}{16}\|q\|^2 \mathbf{Q}(q) \cdot \mathbf{A} \mathbf{Q}(q) - \frac{1}{6}\|q\|^2 \mathbf{L}(q, p) \cdot \mathbf{B} \mathbf{Q}(q) + \dots$$

where

$$\mathbf{L}(q, p) = \mathbf{Q}(q) \times \mathbf{P}(q, p)$$

is the orbital angular momentum. Here we dropped the primes, the hat and the subscript KS: from now on we will only deal with the regularized Hamiltonian, and we also ignored high order terms. Note that (9) is the constant energy scaling. The other possibility is the n -shell scaling. See [1] for more details.

4. Keplerian normal form and reduction. Our main result

In order to descend on $\mathbb{S}^2 \times \mathbb{S}^2$ (through a symplectic reduction procedure) we need first to average H over the flow of H_0 . We obtain the averaged Hamiltonian

$$\mathcal{H} = 2n + \mathcal{H}_2 + \dots$$

In this way H becomes a perturbation on $\mathbb{S}^2 \times \mathbb{S}^2$ of \mathcal{H}_2 which commutes with n and, by the construction outlined in sec. 3, with ζ .

In the KS space $T^*\mathbb{R}^4$ we can have only 6 linearly independent quadratic polynomials in the q and p variables that commute with n and ζ . We can choose these polynomials to be $\mathbf{L} = (L_1, L_2, L_3)$ and $\mathbf{K} = (K_1, K_2, K_3)$ defined as:

$$\begin{aligned} \mathbf{L} &= \frac{1}{2}(\mathbf{q} \times \mathbf{p} + \mathbf{q}p_4 - \mathbf{p}q_4) \\ \mathbf{K} &= -\frac{1}{4}(\mathbf{M}_{\text{KS}}(q)q + \mathbf{M}_{\text{KS}}(p)p) \end{aligned}$$

where $\mathbf{q} = (q_1, q_2, q_3)$ and $\mathbf{p} = (p_1, p_2, p_3)$. They satisfy the relations

$$\begin{aligned} \|\mathbf{L}\|^2 + \|\mathbf{K}\|^2 &= n^2 + \frac{\zeta^2}{4} \\ \mathbf{L} \cdot \mathbf{K} &= -\frac{1}{2}\zeta n. \end{aligned} \tag{10}$$

\mathbf{L} and \mathbf{K} correspond respectively to the orbital angular momentum and to the (rescaled) Runge-Lenz vector for the original Kepler problem.

It is convenient to introduce

$$\mathbf{J}_1 = \frac{\mathbf{L} + \mathbf{K}}{2} \text{ and } \mathbf{J}_2 = \frac{\mathbf{L} - \mathbf{K}}{2}$$

for which relations (10) become

$$\begin{aligned} \|\mathbf{J}_1\| &= \frac{n}{2} + \frac{\zeta}{4} \\ \|\mathbf{J}_2\| &= \frac{n}{2} - \frac{\zeta}{4} \end{aligned}$$

and denoting $\mathbf{J}_\alpha = (J_{\alpha 1}, J_{\alpha 2}, J_{\alpha 3})$

$$\{J_{\alpha i}, J_{\beta j}\} = \delta_{\alpha\beta} \epsilon_{ijk} J_{\alpha k}. \quad (11)$$

This means that \mathbf{J}_1 and \mathbf{J}_2 parametrize a space symplectomorphic to $\mathbb{S}^2 \times \mathbb{S}^2$ equipped with the standard $\mathfrak{so}(4) \cong \mathfrak{so}(3) \oplus \mathfrak{so}(3)$ structure (in particular if the system is defined through a regularization procedure, we have that $\zeta = 0$ and so the radii of the spheres are the same and equal to $n/2$).

Using standard methods of the invariant theory [12, 13], we can show that *any* function that commutes with n and ζ can be written in terms of the components of \mathbf{J}_1 and \mathbf{J}_2 . This implies that the phase space obtained through the symplectic reduction of the \mathbb{T}^2 symmetry generated by n and ζ , on which \mathcal{H}_2 is naturally defined, is $\mathbb{S}^2 \times \mathbb{S}^2$ with the symplectic structure (11).

The expression of \mathcal{H}_2 can be computed by means of standard techniques. The leading order of the perturbation is a homogeneous polynomial of degree 4 in (q, p) times $\|q\|^2$ (due to the regularization procedure). After averaging under the flow of H_0 this gives a quadratic form in the components of \mathbf{J}_1 and \mathbf{J}_2 times n .

There we stop at this principal nontrivial term. We assume homogeneous fields vanishing and we neglect all higher order terms such as the ones produced by second averaging, coming from higher order inhomogeneities, and quadratic Zeeman term.

We can now state our main result. We have found that

$$\mathcal{H}_2 = n \tilde{\mathbf{J}} \cdot \mathbf{M} \tilde{\mathbf{J}} \quad (12a)$$

where $\tilde{\mathbf{J}} = (\mathbf{J}_1, \mathbf{J}_2)$ and \mathbf{M} is the 6×6 matrix:

$$\mathbf{M} = \begin{pmatrix} \mathbf{A} + \mathbf{B} & -\frac{3}{2}\mathbf{A} \\ -\frac{3}{2}\mathbf{A} & \mathbf{A} - \mathbf{B} \end{pmatrix}; \quad (12b)$$

the 3×3 matrices \mathbf{A} and \mathbf{B} are introduced in (9) and depend on the field parameters.

It can be shown that for general fields \mathbf{F} and \mathbf{G} the system with this Hamiltonian \mathcal{H}_2 on $\mathbb{S}^2 \times \mathbb{S}^2$ is not Liouville integrable, see sec. 7. In the subsequent sections, we consider two groups of specific results: the inhomogeneous field is defined purely by the vector potential (sec. 5); the system has an additional axial symmetry (sec. 6). In both cases the system with \mathcal{H}_2 is Liouville integrable.

5. Perturbations by a pure magnetic field

When the field is purely magnetic then matrix $\mathbf{A} = 0$ and the Hamiltonian \mathcal{H}_2 is given by

$$\mathcal{H}_2 = n(\mathbf{J}_1^T \mathbf{B} \mathbf{J}_1 - \mathbf{J}_2^T \mathbf{B} \mathbf{J}_2)$$

If $\mathbf{R} \in \text{SO}(3)$ is an orthogonal transformation that diagonalizes \mathbf{B} , then the canonical transformation defined by

$$(\mathbf{P}, \mathbf{Q}) = (\mathbf{R}\tilde{\mathbf{P}}, \mathbf{R}\tilde{\mathbf{Q}})$$

leaves the Kepler Hamiltonian invariant and induces, on the reduced phase space $\mathbb{S}^2 \times \mathbb{S}^2$, the symplectic change of coordinates

$$(\mathbf{J}_1, \mathbf{J}_2) = (\mathbf{R}\tilde{\mathbf{J}}_1, \mathbf{R}\tilde{\mathbf{J}}_2).$$

In this new coordinate system \mathcal{H}_2 becomes (dropping the tilde from the dynamical variables):

$$\mathcal{H}_2 = n\lambda_1(J_{1,1}^2 - J_{2,1}^2) + n\lambda_2(J_{1,2}^2 - J_{2,2}^2) + n\lambda_3(J_{1,3}^2 - J_{2,3}^2) \quad (13)$$

where λ_1, λ_2 and λ_3 are the eigenvalues of \mathbf{B} . It is not restrictive to consider the situation $\lambda_1 \geq \lambda_2 \geq \lambda_3$ (and $\lambda_1 \neq \lambda_3$, otherwise the traceless matrix \mathbf{B} would be zero). Adding to equation (13) the quantity $n\lambda_3(\mathbf{J}_2^2 - \mathbf{J}_1^2)$, which vanishes on $\mathbb{S}^2 \times \mathbb{S}^2$, and dividing by the positive quantity $2(\lambda_1 - \lambda_3)$ (through a rescaling of time) we obtain

$$\mathcal{H}_2 = n(\mathcal{K}_\lambda(\mathbf{J}_1) - \mathcal{K}_\lambda(\mathbf{J}_2))$$

where

$$\mathcal{K}_\lambda(\mathbf{J}_i) = \frac{J_{i1}^2}{2} + \lambda \frac{J_{i2}^2}{2} \quad i = 1, 2$$

is the Hamiltonian of a rigid rotor on \mathbb{S}^2 and

$$\lambda = \frac{\lambda_2 - \lambda_3}{\lambda_1 - \lambda_3} \in [0, 1].$$

Adding the (constant) quantity $n\|\mathbf{J}_2\|^2$ to \mathcal{H}_2 and performing a rotation around the second axis on the second sphere we have:

$$\mathcal{H}_2 = n(\mathcal{K}_\lambda(\mathbf{J}_1) + \mathcal{K}_{1-\lambda}(\mathbf{J}_2)).$$

From these expressions it is straightforward to conclude that, no matter what the field parameters are, \mathcal{H}_2 is integrable, being the sum of two uncoupled 1-degree of freedom systems. The anisochronicity of \mathcal{K}_λ , moreover, implies the anisochronicity of \mathcal{H}_2 .

5.1. Convexity properties

Since \mathcal{H}_2 is integrable its local representatives are functions of the local actions only. Along with the anisochronicity of the motions it is interesting to verify the convexity in the actions §. This plays a crucial role when higher order terms of \mathcal{H} are taken into account. In this case the system is no longer Liouville integrable but it is, in fact, a perturbation of \mathcal{H}_2 . Through Nekhoroshev theory it is possible however to prove, under convexity assumptions on \mathcal{H}_2 and provided that the perturbation is small enough, that the dynamics of the action variables is bounded over an exponentially long time scale. See [14] for a detailed account on Nekhoroshev theory.

§ A polynomial function \mathcal{H}_2 in the two (local) actions is convex if its second derivative \mathcal{H}_2'' is a positive definite quadratic form. Note, however, that the concept of convexity can be defined without employing the local representatives.

We prove that in the case of the presence of an axially symmetric magnetic field ($\lambda = 0$) there is no convexity in the actions, while in the non-axially symmetric case, a generic linear magnetic field provides convexity (at least in a region of the phase space). Therefore, such systems are suitable for studying quantum manifestations of Nekhoroshev stability, a widely acknowledged aspect of classical dynamics which has not yet been observed in the quantum world (a first step toward this has been done in [15]).

5.1.1. Special non-convex case When $\lambda = 0$ (the field is axially symmetric), $\mathcal{H}_2 = n(J_{11}^2 - J_{21}^2)$. When $2J_{i1} \neq \pm n$ for $i = 1, 2$, J_{11} and J_{21} are valid action variables for the system and we have that the Hessian matrix of \mathcal{H}_2 is

$$\mathcal{H}_2''(\mathbf{J}_1, \mathbf{J}_2) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

showing that the system is non-convex. An equivalent situation arises when $\lambda = 1$.

5.1.2. Convexity in the non-axially symmetric case When $\lambda \in (0, 1)$, \mathcal{K}_λ admits a separatrix which defines four disjoint regions on \mathbb{S}^2 where action-angle coordinates should be constructed separately.

Just as for the reduced Euler top, an explicit expression for the action in terms of elementary functions is not possible. It is, however, possible to give an expression for the period of the system as a function of the energy. Let h be the energy (with a slight abuse of notation we will identify both the energy value and the Hamiltonian with h). Supposing $0 \leq 8h < \lambda n^2$ it is can be shown that (an analysis of the dynamics of the Hamiltonian \mathcal{K}_λ can be found for example in [16]):

$$T(h) = \frac{8n}{\sqrt{\lambda(n^2 - 8h)}} K \left(\frac{8h(1 - \lambda)}{\lambda(n^2 - 8h)} \right)$$

where $K(m)$ is the complete elliptic integral of the first kind. The action can be expressed as a function of the energy

$$I(h) = \frac{1}{2\pi} \int_0^h T(\Sigma) d\Sigma$$

and the Hamiltonian, as a function of the action, can be found by inverting $I(h)$. It is possible to express the frequency map $\omega = h'$ as a function of the energy through the relation:

$$\omega(I(h)) = \frac{2\pi}{T(h)}.$$

To compute the Hessian $M = h''$ of the Hamiltonian with respect to the actions, we use the formula that relates the second derivative of a function with the one of its inverse:

$$M(I(h)) = -4\pi^2 \frac{T'(h)}{T^3(h)}.$$

The case $\lambda < 8hn^{-2} \leq 1$ can be analysed in an analogous way by employing the substitution $(h, \lambda) \rightarrow (\frac{n^2}{8} - h, 1 - \lambda)$.

Using the fact that

$$K'(m) = \frac{E(m) - (1-m)K(m)}{2m(1-m)},$$

where $E(m)$ is the elliptic integral of the second kind (a standard expression that can be found, for instance, in [17]), introducing the function

$$x = x(h) = \frac{8h(1-\lambda)}{(n^2 - 8E)\lambda} \in [0, 1].$$

it is possible to see that

$$M(I(h)) = \frac{\pi^2}{4n^2} \frac{(1-x)(1-\lambda)K(x) - (1-(1-x)\lambda)E(x)}{(1-x)xK(x)^3} \quad (14)$$

From this expression it is possible to check that (I_{\max} here is the value of the action at the separatrix)

$$M(0) = -\frac{1+\lambda}{2n^2}$$

$$\lim_{I \rightarrow I_{\max}} M(I) = -\infty$$

If we want to prove that $M(I)$ is negative for $I \in [0, I_{\max})$, it is sufficient to prove that M is a decreasing function. From an analysis of the zeros of its derivative, it can be seen that any critical point of M in the interval $x = x(h(I)) \in (0, 1)$, corresponds to a zero of

$$P(x) = 3E(x)^2 - 2(2-x)E(x)K(x) + (1-x)K(x)^2.$$

Now that any dependence from λ has been factored out, it is a matter of standard analysis to show that $P(x)$ does not possess zeros for $x \in (0, 1)$. These calculations show that, for $8h(I) < \lambda n^2$,

$$M(I) \leq -\frac{1+\lambda}{2n^2} < 0,$$

while for $8h(I) > \lambda n^2$ we have

$$M(I) \geq \frac{2-\lambda}{2n^2} > 0.$$

Back to the original system, the actions for \mathcal{H}_2 are defined in a straightforward way from the actions for the two rotors. In particular around each minimum and each maximum of \mathcal{H}_2 on $\mathbb{S}^2 \times \mathbb{S}^2$ we have that the Hessian of \mathcal{H}_2 is bounded away from zero:

$$\|\mathcal{H}_2''\| \geq \frac{1 + \min(\lambda, 1-\lambda)}{2n^2} > 0$$

and so the Hamiltonian is convex (in other regions^{||}, however, \mathcal{H}_2'' is not positive defined and so there \mathcal{H}_2 is not convex).

^{||} There are sixteen disjoint connected regions on $\mathbb{S}^2 \times \mathbb{S}^2$, each one defined as the product of a region containing a maximum or a minimum on \mathbb{S}^2 of the Hamiltonians \mathcal{K}_λ and $\mathcal{K}_{1-\lambda}$. \mathcal{H}_2 is convex in the eight zones related to the pairs of maxima or minima.

6. Perturbations by an axially symmetric field

Generally, when an electric field is present, there are no simple integrals of motion. An exceptional case is encountered when an electromagnetic field is invariant under any rotation around a fixed axis. In this case, there exists a non-zero $\mathbf{W} \in \mathbb{R}^3$ and $\mathbf{R} \in \text{SO}(3)$ such that:

$$\begin{aligned}\mathbf{R}\mathbf{W} &= \mathbf{W} \\ \mathbf{R}\mathbf{F}(\mathbf{Q}) &= \mathbf{F}(\mathbf{R}\mathbf{Q}) \\ \mathbf{R}\mathbf{G}(\mathbf{Q}) &= \mathbf{G}(\mathbf{R}\mathbf{Q}).\end{aligned}$$

By a suitable choice of the reference frame, it is not restrictive to consider the case $\mathbf{W} = (1, 0, 0)^T$. In this way, we can find constants α and β such that

$$\begin{aligned}\mathbf{A} &= \frac{\beta}{3} \text{diag}(2, -1, -1) \\ \mathbf{B} &= \frac{\alpha\beta}{3} \text{diag}(2, -1, -1).\end{aligned}$$

Having already analysed the purely magnetic case $\mathbf{A} = 0$, we can, after a reparametrization of time, let $\beta = 1$.

With all these simplifications the averaged Hamiltonian (12a) becomes:

$$\mathcal{H}_2 = n \left(K_1^2 + \frac{\xi}{4} + \alpha K_1 L_1 - \frac{n^2}{6} \right) \quad (15)$$

where

$$\xi = 4(\mathbf{J}_1 \cdot \mathbf{J}_2 - J_{11}J_{21}) = \mathbf{L}^2 - \mathbf{K}^2 - (L_1^2 - K_1^2).$$

A consequence of the invariance of the original system is the invariance of \mathcal{H}_2 under simultaneous rotations around the first axes on the two spheres. Furthermore,

$$\{\mathcal{H}_2, L_1\} = 0.$$

Since we are dealing with a two degree of freedom system this implies that \mathcal{H}_2 defines a Liouville integrable system on $\mathbb{S}^2 \times \mathbb{S}^2$.

In order to study the geometry of the family of tori of our present system (i.e. of the integrable fibration) we use reduction of the \mathbb{S}^1 symmetry action. Since similar analysis can be found elsewhere (see for example [6]), we do it very briefly. We also should note that, the n -shell energy-momentum diagrams in this section and the particular degeneracy patterns can be observed experimentally (by measuring the energies of the quantum states and finding their quantum number m of the angular momentum projection).

6.1. Reduction of the axially symmetric case

Since \mathcal{H}_2 is invariant under the Hamiltonian \mathbb{S}^1 action generated by L_1 it is convenient to perform the symplectic reduction relative to this action. A generic L_1 -invariant Hamiltonian can be written as a function of L_1 , K_1 , ξ and σ , where

$$\sigma = 2(L_2K_3 - L_3K_2) = 4(J_{22}J_{13} - J_{12}J_{23}).$$

These four invariants satisfy the relation

$$\sigma^2 + \xi^2 - ((n + L_1)^2 - K_1^2)((n - L_1)^2 - K_1^2) = 0. \quad (16)$$

For a fixed value m of L_1 , equation (16) defines a (possibly singular) symplectic manifold \mathcal{R}_m and the reduction procedure associating to any invariant Hamiltonian on $\mathbb{S}^2 \times \mathbb{S}^2$ a reduced Hamiltonian on \mathcal{R}_m .

For $m \neq 0, \pm n$, \mathcal{R}_m is a two-dimensional differentiable manifold diffeomorphic to \mathbb{S}^2 , whose each point is lifted to a generic circular orbit of the \mathbb{S}^1 action. For $m = \pm n$, \mathcal{R}_m reduces to a point and the orbits of the action are the fixed points $\mathbf{K} = \mathbf{0}$, $\mathbf{L} = (\pm n, 0, 0)^T$. \mathcal{R}_0 is homeomorphic to \mathbb{S}^2 , but the reduction relative to the points $\sigma = \xi = 0$, $K_1 = \pm n$ is singular and the orbits of the action above these points are the fixed points $\mathbf{L} = \mathbf{0}$, $\mathbf{K} = (\pm n, 0, 0)^T$. Naturally, the four isolated fixed points are the equilibria of \mathcal{H}_2 on $\mathbb{S}^2 \times \mathbb{S}^2$.

6.2. Analysis of the invariant fibration in the reduced phase space

The system with Hamiltonian \mathcal{H}_2 can be regarded as an integrable system on the (at most) two-dimensional phase space \mathcal{R}_m . The geometry of the corresponding invariant (singular) fibration is defined by the level sets of \mathcal{H}_2 , see the typical example in fig. 1 and the explanation below. The analysis is quite simple and easy to follow. It relies on classifying intersections in \mathbb{R}^3 of the sphere-like shape \mathcal{R}_m with cylindrical (in σ) level sets of \mathcal{H}_2 .

When \mathcal{H}_2 is a submersion, and \mathcal{R}_m is nonsingular, the regular fibres are, by the Liouville-Arnol'd theorem, the disjoint unions of one-dimensional tori, while the connected components of the critical fibres represent equilibria or separatrices of the system. When \mathcal{H}_2 is defined by (15), the regular fibres can either be connected or have two connected components. At critical energies separating regular energy intervals, we find invariant fibres with a different number of connected components. These critical fibres can be of two kinds:

- (i) The fibre is connected and contains a hyperbolic fixed point for the flow of \mathcal{H}_2 : it resembles a figure eight and represents a separatrix of the reduced system;
- (ii) At least one of the connected components of the fibre is an elliptic fixed point for the flow of \mathcal{H}_2 .

On \mathcal{R}_m , when $|m| < n$ (the case $|m| = n$ is trivial), \mathcal{H}_2 possesses a single global minimum (elliptic fixed point) and so for “low” energies the invariant fibres are connected. If m is large enough (i.e. $|m| > m_\alpha$ for some $m_\alpha \in (0, n)$, depending on the value of α), then *all* fibres are connected and the only other critical fibre is the global maximum (an elliptic fixed point). If, on the other hand, m is close to 0 (fig. 1), then a hyperbolic fixed point with a corresponding eight-shaped singular fibre (yellow line in fig. 1) are present, and at energies higher than that of this fibre, we have a continuous family of disconnected regular fibres. If $\alpha = 0$, then there is only one more critical fibre which corresponds to the global maximum of the energy and which is a disjoint union of two elliptic fixed points. If $\alpha \neq 0$ (fig. 1), we have a local maximum of the energy corresponding to the disjoint union of a circular orbit and a fixed point followed by the global maximum which corresponds to a single fixed point.

To compute the energy values at the critical fibres on \mathcal{R}_m it is sufficient to find the values of (K_1, ξ, σ) for which

$$c(K_1, \xi, \sigma) = \xi^2 + \sigma^2 - ((n - m)^2 - K_1^2)((n + m)^2 - K_1^2) = 0$$

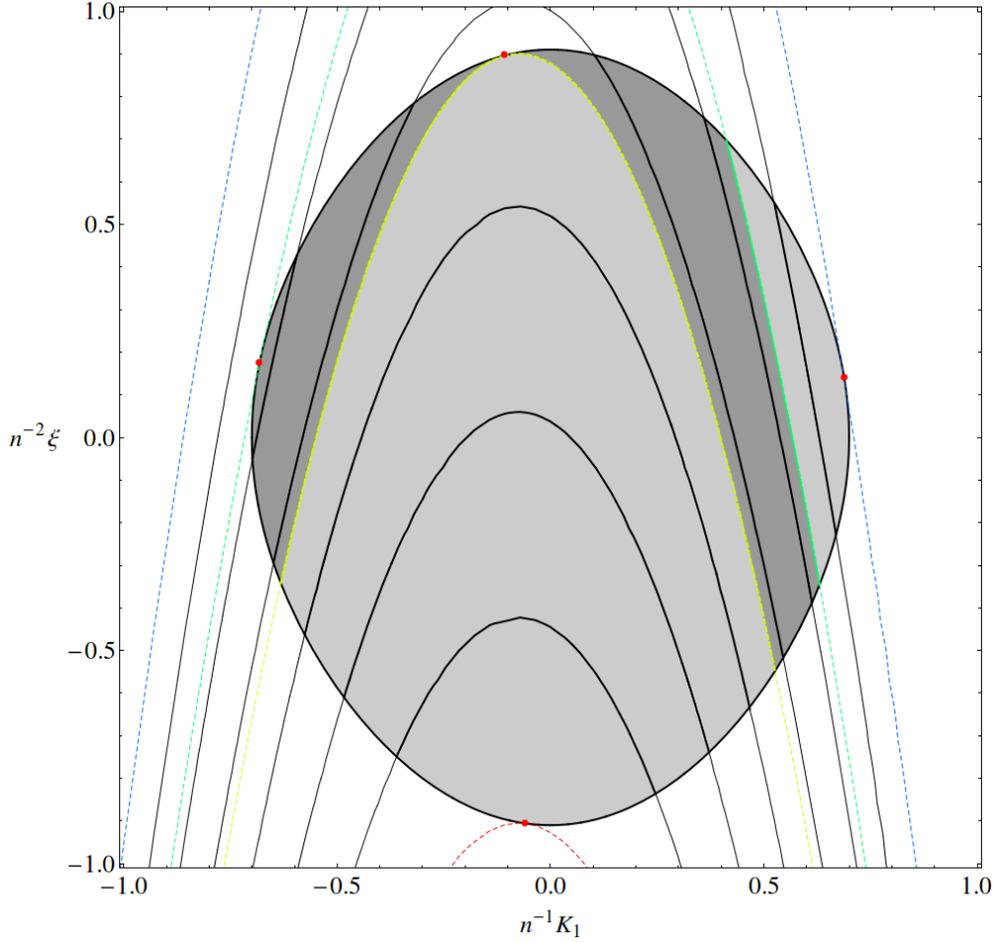


Figure 1. Constant energy level sets and the reduced phase space for $L_1 = 0.3$ and $\alpha = .5$ shown in the projection on the $\sigma = 0$ plane with coordinates (ξ, K_1) . The image of the reduced phase space $\mathcal{R}_{0.3}$ is shaded gray. Each line represents a level set of \mathcal{H}_2 ; bold lines mark the intersection with $\mathcal{R}_{0.3}$. Continuous black and coloured lines represent regular and critical fibres, respectively. Critical points of \mathcal{H}_2 on $\mathcal{R}_{0.3}$ are shown in red. In the light grey area we have connected regular fibres; in the dark grey area, we have fibres with two connected components.

and such that $d\mathcal{H}_2(K_1, \xi, \sigma) \wedge dc(K_1, \xi, \sigma) = 0$. Calculations are greatly simplified by the fact that \mathcal{H}_2 does not depend on σ and consequently for any critical point we have $\sigma = 0$. This leads to equations

$$\begin{aligned} K_1^3 + 4\xi K_1 - (m^2 + n^2)K_1 + 2\alpha m\xi &= 0 \\ \xi^2 - ((n - m)^2 - K_1^2)((n + m)^2 - K_1^2) &= 0, \end{aligned}$$

which can be rewritten as $\xi = P(K_1)$ and $Q(K_1) = 0$ where polynomials P and Q depend parametrically on m , n , and α . The solutions of this system give the critical points of \mathcal{H}_2 and the corresponding critical fibres. The discriminant $\Delta(m)$ of Q is a polynomial that depends parametrically on α . This polynomial has one real root m_α in

the open interval $(0, n)$. This threshold value m_α signals the existence of disconnected regular invariant fibres for $|m| < m_\alpha$.

6.3. Analysis of the invariant fibration on $\mathbb{S}^2 \times \mathbb{S}^2$

It is straightforward to extend the previous analysis in order to describe the invariant singular fibration defined by \mathcal{H}_2 on $\mathbb{S}^2 \times \mathbb{S}^2$. For $0 < |m| < n$, the connected components of any regular fibre lift to two-dimensional tori, the elliptic points lift to periodic orbits and the eight-shaped fibres lift to bitorus (two two-dimensional tori “glued” together on a circle). For $|m| = 0$, the situation is the same, except for the fibre that contains only the two singular points of \mathcal{R}_0 (and that corresponds to the global maximum of \mathcal{H}_2). The corresponding fibre on $\mathbb{S}^2 \times \mathbb{S}^2$ is a disjoint union of two fixed points. Finally, in the case $|m| = n$, the single invariant fibre is lifted to a fixed point on $\mathbb{S}^2 \times \mathbb{S}^2$.

6.4. The energy-momentum map and the quantum lattice

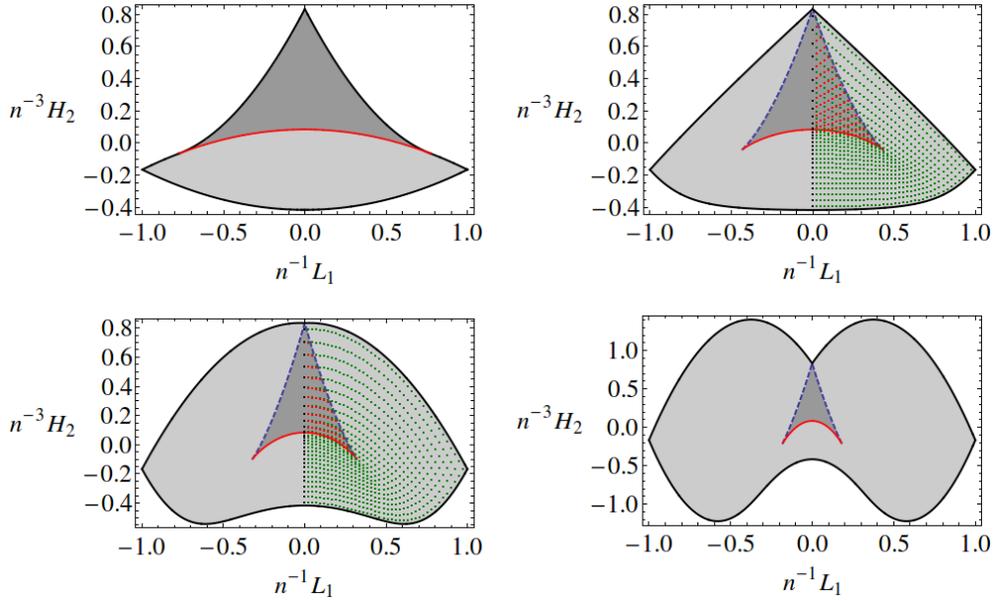


Figure 2. Energy momentum map for the axially symmetric system for $\alpha = 0, 1, 2, 5$. Lines mark critical fibres. Specifically, solid black lines represent periodic orbits, red solid lines correspond to bitorus, while blue dashed lines mark disjoint unions of a torus and a periodic orbit. Over the light gray area the fibres are connected, while over the darker area the fibres have two connected components. For $\alpha = 1, 2$ the lattice of the quantum spectrum is also given (for $L_1 \geq 0$ only, since the picture is symmetric for negative values). Each point represents an eigenstate of the system, the colors are related to the expectation value $\langle K_1 \rangle$: green if it is greater than \bar{k} , red if it is smaller to \bar{k} , and black if it is equal to \bar{k} , where \bar{k} is the projection on the K_1 axis of the critical point of \mathcal{H}_2 relative to the bitorus (or to the global maximum if the former is not present).

To describe globally the invariant foliation on $\mathbb{S}^2 \times \mathbb{S}^2$ generated by \mathcal{H}_2 we consider

the energy-momentum map

$$\mathcal{EM} : \mathbb{S}^2 \times \mathbb{S}^2 \rightarrow \mathbb{R}^2 : x \mapsto (L_1(x), \mathcal{H}_2(x)).$$

The fibres of \mathcal{EM} are the invariant sets of the system which are found as described in the previous sections for varying fixed values m of L_1 . The image of \mathcal{EM} is illustrated in fig. 2. In the plane parametrized by the values of \mathcal{EM} , the images of the critical fibres (bitori and periodic orbits) are highlighted, while the regular domains where each point lifts to the same number of connected components \mathbb{T}^2 (one or two) are distinguished using different colors.

We notice two qualitatively different situations. When $\alpha \neq 0$ there is a triangular region, over which we have regular fibres with two connected components. The lower boundary of this domain is a curve representing bitori, the lateral boundaries lift to the disjoint union of a two-dimensional torus and a periodic orbit. Surrounding this region is another larger region where each point lifts to one connected regular fibre, and whose boundaries represent families of periodic orbits (global maxima/minima of the reduced system). It is interesting to observe that it is possible to “cross” the lateral boundaries of the first (inner) region. Specifically, it is always possible to lift any given path in the (L_1, \mathcal{H}_2) plane which crosses the lateral boundaries to $\mathbb{S}^2 \times \mathbb{S}^2$ in a way that the singular fibres are avoided, but this is not possible if the path crosses the lower boundary. When $\alpha = 0$ (purely electric field) the lateral boundaries of the inner region merge with the boundaries of the outer one dividing the fibration in two disconnected zones whose common boundary cannot be crossed.

In the presence of regular disconnected fibres, we can represent the image of the \mathcal{EM} as a two-sheeted (two cell) *unfolding surface* (see the discussion in [1, 18]), with a smaller triangular sheet (or lower cell, dark gray in fig. 2) glued to the larger sheet along the bitorus line. Regular points in each sheet (or cell) lift to a single regular torus \mathbb{T}^2 . When the bitorus line is isolated within the larger sheet (larger lower cell, light gray), the system has monodromy for any path encircling this bitorus line (cf for example [19]).

It is interesting to observe also how the geometry of the system is reflected in the quantum analogue. The Hamiltonian \mathcal{H}_2 can be quantized in a standard way [20]. The joint spectra of $\hat{\mathcal{H}}_2$ and \hat{L}_1 (the quantized projection of the angular momentum with quantum number m) defines a lattice in \mathbb{R}^2 , see fig. 2. This lattice follows the lines of constant classical local actions of the system and shows a clear near degeneracy in the smaller triangular sheet of the stratified \mathcal{EM} image. To distinguish the lower and the upper sheets, observe that classically, for a given value of L_1 admitting disconnected regular fibres (cf fig. 1, dark gray shade), there exists $\bar{k} \in (-n, n)$ such that the connected components of the fibre, in the inner sheet, are characterized either by $K_1 < \bar{k}$ or $K_1 > \bar{k}$ (\bar{k} is the K_1 -component of the hyperbolic point). In the quantum case we can classify the eigenstates of \mathcal{H}_2 by their expectation value of the quantum observable corresponding to K_1 (with respect to the value of \bar{k}). As illustrated in fig. 2, we can distinguish in this way the different sublattices and in particular, that one family (green dots in fig. 2) can be defined on the whole EM image (both inside and outside the inner region) in a regular way, enforcing the idea that the singular lines in the EM image caused by the elliptic points are crossable. It should be noted that this distinction of sublattices can be done only if there is no additional reversal symmetry $K_1 \leftrightarrow -K_1$ (which is present in the case $\alpha = 0$ or when $L_1 = 0$).

7. The general case: non-integrability

In the general case, when the system possesses no extra axial symmetry and an inhomogeneous electric field is present, no simple integrals of motions seem to exist. While proving non-integrability, i.e., excluding the existence of a function f on $\mathbb{S}^2 \times \mathbb{S}^2$ which is functionally independent from \mathcal{H}_2 and which Poisson commutes with \mathcal{H}_2 ,

$$\{f, \mathcal{H}_2\} = 0,$$

may be difficult (cf [7]), strong indications can be given.

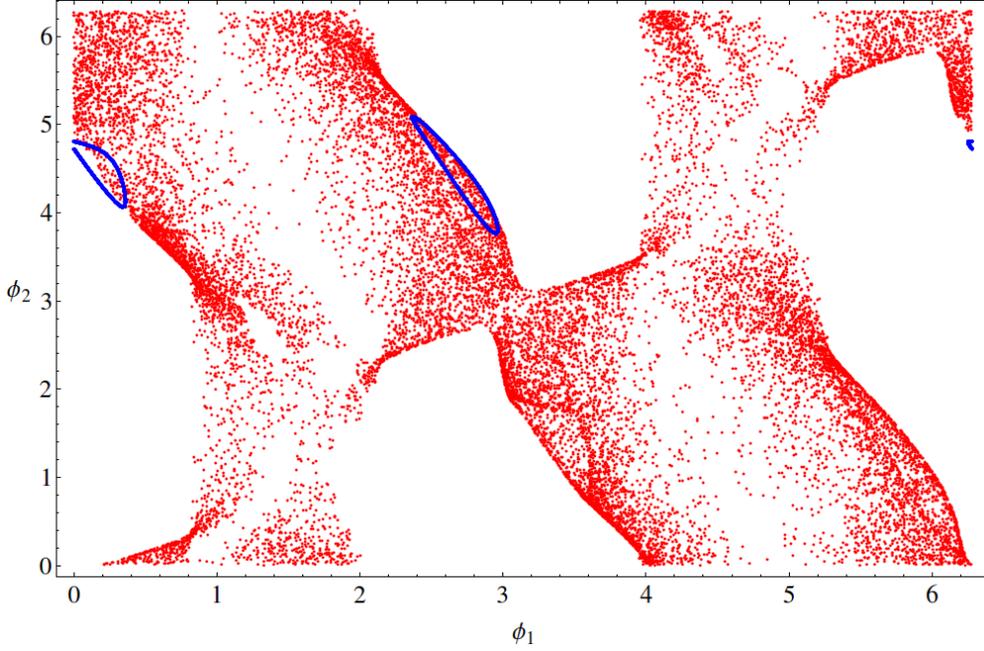


Figure 3. Poincaré sections for two orbits (blue and red points) launched at the same energy for a generic field configuration. The surface of section is defined by $J_{11} = 0$ with coordinates given by the polar angles ϕ_1 and ϕ_2 corresponding to axes J_{11} and J_{21} . The blue orbit is regular; the red orbit clearly exhibits a chaotic behaviour.

In particular, it is possible to check systematically for the presence (or absence) of polynomial first integrals of a given maximal degree in the \mathbf{J} components. Let p_1, \dots, p_k and q_1, \dots, q_l be the bases for the polynomials with given maximal degrees d and $d + 1$ respectively. Since \mathcal{H}_2 is quadratic we have:

$$\{p_i, \mathcal{H}_2\} = \sum_j P_{ij} q_j,$$

where P is a matrix with real entries. For any element $\mathbf{w} = (w_1, \dots, w_k)$ in the kernel of P we can define $f = \sum_i w_i p_i$ satisfying

$$\{f, \mathcal{H}_2\} = 0.$$

So the task of finding a polynomial integral of motion f is reduced to finding the kernel of P . Note that we should exclude from the kernel of P any “trivial”

invariant polynomial which can be obtained by combination (through addition and multiplication) of \mathcal{H}_2 and the Casimirs of the system. It is always possible to suppose that p_{m+1}, \dots, p_k define, for some $m < k$, a basis for the “trivial” part of the kernel and then it is sufficient to consider only linear combinations of p_1, \dots, p_m .

At this point, if \mathcal{H}_2 is non-integrable then matrix \mathbf{P} has maximum rank for every d . When the dependence on the field parameters is restored, \mathbf{P} becomes a matrix depending (linearly) on the parameters and the kernel is nontrivial for a given field configuration if the determinant (which is a multivariate polynomial in the field parameters) of any $m \times m$ submatrix of \mathbf{P} vanishes for the corresponding parameters. In general, using a Gröbner basis algorithm with a good choice of a limited number of submatrices, it is possible to prove the polynomial non-integrability of the system. Thus for example, we can show that *any system that admits linear integrals is axially symmetric*.

For a purely electric inhomogeneous field, it is possible to find a basis in which the matrix \mathbf{A} is diagonal and, after rescaling \mathcal{H}_2 , to see that the system depends essentially on only one parameter. In this way the determinant of any square submatrix of \mathbf{P} is made a polynomial in one variable with only a finite number of roots that can be examined by hand (or it is sufficient to check if different submatrices determine polynomials with common roots). In particular, we have verified that there are no polynomial invariants up to maximal degree 4.

Another way to demonstrate non-integrability, for a given field configuration but without any restriction to the class of possible invariants, is to uncover the irregular motion through numerical integration. An example is given in fig. 3 where one orbit, shown in blue, is picked sufficiently close to an elliptic equilibrium and remains on a KAM torus, while the other orbit, in red, is visibly chaotic. The computations in fig. 3 were done for a generic inhomogeneous fields configuration with

$$A = \begin{pmatrix} 2 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & -4 \end{pmatrix}, \text{ and } B = \begin{pmatrix} -2 & 1 & -1 \\ 1 & -2 & -2 \\ -1 & -2 & 4 \end{pmatrix}.$$

8. Energy of the perturbed system and concrete applications

A drawback of Kustaanheimo-Stiefel regularization, which may be problematic in applications, is that the expressions for the Hamiltonian contain, through Ω , the (perturbed) energy of the system as a parameter instead of the principal quantum number n . The procedure to extract energy from the Kustaanheimo-Stiefel normal form is described in [1]. We briefly discuss here the necessary modifications that should be employed in our case (which is relatively simple since we only use the first order average).

The basic idea is that we can express the perturbed energy E as

$$E = -\frac{1}{2n^2} + \Delta E, \quad (17)$$

where the first term is the unperturbed Keplerian energy and ΔE is the so called energy correction. In particular we have that (ignoring high order terms in ΔE)

$$4H_{\text{KS}} = \Omega^{-1} = \frac{1}{\sqrt{-8E}} = \frac{n}{2} + \frac{n^3}{2}\Delta E + o(\Delta E). \quad (18)$$

In the first order approximation, we obtain from (18) that

$$H_{KS} = 2n + 2n^3 \Delta E \quad (19a)$$

Furthermore we can define the n -scaled analogs of (9)

$$\mathbf{A} = \frac{n^4}{2} \mathbf{F} \quad \text{and} \quad \mathbf{B} = -\frac{3n^3}{8} \mathbf{G}, \quad (19b)$$

and from (19a) we obtain

$$\Delta E = \frac{1}{2n^3} (H_{KS} - 2n) \quad (20)$$

Averaging ΔE we obtain the Hamiltonian

$$\overline{\Delta E} = \Delta \mathcal{H}_2 = \frac{1}{2n^2} \tilde{\mathbf{J}} \cdot \mathbf{M} \tilde{\mathbf{J}}, \quad (21)$$

where \mathbf{M} is the same that has been already defined in (12b) except that the new expressions (19b) for \mathbf{A} and \mathbf{B} in terms of n should be used. The first order normal form approximation of the in order to compute the energy, is obtained by adding the unperturbed keplerian energy (in terms of n):

$$\mathcal{H} = -\frac{1}{2n^2} + \Delta \mathcal{H}_2 = -\frac{1}{2n^2} (1 - \tilde{\mathbf{J}} \cdot \mathbf{M} \tilde{\mathbf{J}}). \quad (22)$$

For example, let us consider the magnetic case with $\mathbf{F} = 0$. We have that

$$-\tilde{\mathbf{J}} \cdot \mathbf{M} \tilde{\mathbf{J}} = \frac{3n^3}{8} (\mathbf{J}_1 \cdot \mathbf{G} \mathbf{J}_1 - \mathbf{J}_2 \cdot \mathbf{G} \mathbf{J}_2).$$

Recall that \mathbf{G} is the 3×3 symmetric traceless matrix defining the nonhomogeneous (linear) magnetic field $\mathbf{G}(\mathbf{Q}) = \mathbf{G} \mathbf{Q}$ (See section 2). If we put ourselves in a reference frame where \mathbf{G} is diagonal, that is

$$\mathbf{G}(\mathbf{Q}) = (\lambda_1 x, \lambda_2 y, \lambda_3 z)^T, \quad \lambda_1 + \lambda_2 + \lambda_3 = 0, \quad \lambda_1 \geq \lambda_2 \geq \lambda_3,$$

we have (using the results of Section 5) that the energy

$$-\tilde{\mathbf{J}} \cdot \mathbf{M} \tilde{\mathbf{J}} = \alpha (\mathcal{K}_\beta(\mathbf{J}_1) - \mathcal{K}_\beta(\mathbf{J}_2))$$

with

$$\mathcal{K}_\beta(\mathbf{J}_i) = \frac{1}{2} (J_{i1}^2 + \beta J_{i2}^2), \quad \alpha = \frac{3}{4} n^3 (2\lambda_1 + \lambda_2) \quad \text{and} \quad \beta = \frac{\lambda_1 + 2\lambda_2}{2\lambda_1 + \lambda_2}, \quad (23)$$

is the sum of energies of two rigid rotors.

Since the spectrum of $\mathcal{K}_\beta(\mathbf{J}_i)$, $i = 1, 2$ is nonnegative and bounded from above by $\frac{1}{2} \|\mathbf{J}_i\|^2 = \frac{n^2}{8}$, an estimation for the splitting relative to the keplerian energy due to the perturbation is given by

$$|2n^2 \Delta \mathcal{H}_2| \leq \frac{3}{32} n^5 (2\lambda_1 + \lambda_2).$$

This shows that, in order to justify the perturbative regime, we should require

$$\frac{3}{32} n^5 (2\lambda_1 + \lambda_2) \ll 1 \quad \text{and therefore} \quad 2\lambda_1 + \lambda_2 \ll \frac{32}{3} n^{-5}.$$

Notice that here the field parameters λ_i are in atomic units.

9. Discussion. Specifics of the physical realisation

The fact that *any* perturbation of the hydrogen atom by a sufficiently weak spatially inhomogeneous magnetic field without (or with a very small) homogeneous component is equivalent—in the n -shell approximation—to a nearly integrable system of two identical Euler tops with conserved angular momenta of equal length $\|\mathbf{J}_1\| = \|\mathbf{J}_2\| = n/2$ coupled through higher order terms (sec. 5), a system that is isochronous and generally convex, is certainly a nontrivial and interesting result. It can be very interesting to observe experimentally the fine structure of the n -shell energy levels corresponding to this case. And when such observation become possible, interesting and new phenomena can be studied, notably the Nekhoroshev stability [15].

It is, therefore, pertinent to discuss whether and how such perturbation can be indeed achieved physically. In comparison to the case of homogeneous fields, a number of new challenging difficulties is evident. First of all, the fields should be inhomogeneous on the scale of the classical orbit with Keplerian action $n\hbar$ while the homogeneous component should be excluded (or at least made smaller than the inhomogeneous part). Secondly, the position of the atom with regard to the created field becomes also critical on the same scale. We hope however that contemporary experimental techniques are or will soon become capable of solving these problems.

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¶ Note that n can be quite high in modern experiments, see [21–23]. The size of the orbit is estimated by the n -th Bohr's radius $n^2 a_0$ with $a_0 = \hbar^2 / (m_e e^2) = 0.529 \text{Å}$.

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