Most Typical 1:2 Resonant Perturbation of the Hydrogen Atom by Weak Electric and Magnetic Fields

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We study a perturbation of the hydrogen atom by small homogeneous static electric and magnetic fields in a specific mutual alignment with angle approximately $\pi/3$ which results in the 1:2 resonance of the linearized Keplerian n-shell approximation. The bifurcation diagram of the classical integrable approximation has for most such field configurations the same typical structure that we describe. The structure of the corresponding quantum energy spectrum, which we describe in detail, is in certain ways an analogue of the well-known degeneracy found by Herrick [Phys. Rev. A **26**, 323 (1982)] for the quadratic Zeeman effect.

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Introduction.—With minor simplifications, the hydrogen atom in weak static electric and magnetic fields is a specific perturbation of the Kepler system of two bodies. Pauli [1] recognized the importance of this system to quantum mechanics and atomic physics and came up with a first order analysis which is carried out at the level of the linearization of the Keplerian average of the perturbation. Herrick [2] and Solov'ev and co-workers [3–5] laid the foundation of the second order theory.

Our system is described using integrable approximations with three first integrals that include the energy E and the Keplerian action N; the latter is the classical analogue of the principal quantum number n and for the unperturbed system $E = -1/(2N^2)$. The third integral μ depends essentially on the external fields configuration, as we explain later. The integrals N and μ are often called momenta (because they generate a rotation in appropriate coordinates in the phase space $\mathbb{R}^6$) and the map $\mathcal{EM} = (N, \mu, E):\mathbb{R}^6 \to \mathbb{R}^3$ that assigns to each point in the phase space $\mathbb{R}^6$ the values of the integrals is called the energy-momentum map.

The basic tool for understanding the classical dynamical behavior of the system is the stratified image of $\mathcal{EM}$, or bifurcation diagram. In the bifurcation diagram we depict the physically accessible values (n, m, e) of $\mathcal{EM}$, and we distinguish such values based on the topological type of the fiber of $\mathcal{EM}$ at (n, m, e), i.e., of the common level set $\{N = n, \mu = m, E = e\}$. Such fibers are typically three-dimensional tori $\mathbb{T}^3$ or unions of such tori. In the bifurcation diagram the emphasis is on the nontypical (critical) fibers since they affect the global dynamical properties of the system and the structure of its energy spectrum.

A recent advancement in the understanding of such systems has been the uncovering of resonances of the linearized Keplerian n-shell approximation in Ref. [6] and independently in Ref. [7]. In the latter work the concept of resonance zones was introduced to describe systems near an exact resonance.

Presently, systems which are well understood dynamically (at the level of their integrable approximations) include the two single field limits (Stark and Zeeman effect) and practically all (near-)orthogonal configurations [7–9]. The latter constitute the 1:1 resonance zone. Despite studies of other field configurations [10] our understanding of them remains incomplete.

Results.—Compared to the 1:1 zone, the 1:2 zone corresponds to the next most important resonance, and it is expected and has been found to contain more dynamically complex systems [7] due to the higher order of the resonance.

In this Letter we report that although the dynamical behavior of systems in 1:2 resonance is more complicated compared to systems in the 1:1 zone, nevertheless there is a typical 1:2 resonant system. Thus we observe that for most values of the parameters the stratified image of the (classical) energy-momentum map and the corresponding (quantum) energy spectrum have a specific structure that we describe in detail. The typical quantum n-shell energy spectrum is presented.

Systems with such structure have generalized good quantum numbers and corresponding global action coordinates and we explain how the latter are introduced in the quantum energy spectrum. The existence of global action coordinates is not ensured even if the system is integrable. The hydrogen atom in near-orthogonal fields has monodromy [8] and thus no global action-angle coordinates for many field configurations.

Hamiltonian and parameters.—Let $\mathbf{F} = (F_b, F_e, 0) = -\mathbf{E}$ and $\mathbf{G} = (G, 0, 0) = -|e|\mathbf{B}$ represent the electric field $\mathbf{E}$ and the magnetic flux density $\mathbf{B}$. Without the center of

mass, spin, and relativistic corrections, the Hamiltonian of our system is (in atomic units)

$$H_{3D} = \frac{1}{2}\mathbf{P}^2 - |\mathbf{Q}|^{-1} + F_e Q_2 + F_b Q_1 + \frac{1}{2}G(Q_2 P_3 - Q_3 P_2) + \frac{1}{8}G^2(Q_2^2 + Q_3^2) = E, \quad (1)$$

where $(\mathbf{Q}, \mathbf{P})$ are canonical coordinates on $\mathbb{R}^6$. For a given value $n \geq 0$ of the Keplerian integral N, we introduce the n-scaled field amplitudes $g = Gn^2$, and $f = (f_e, f_b) = 3(F_e, F_b)n^3$ and related field configuration parameters [7,8,11],

$$a^2 = \frac{g^2}{s^2}, \qquad d = \frac{g f_b}{s^2}, \qquad s = \sqrt{g^2 + f_b^2 + f_e^2} \geq 0, \quad (2a)$$

where the combined field strength s is a universal small parameter. For the angle α between $\mathbf{G}$ and $\mathbf{F}$, we have

$$(\tan\alpha)^2 = F_e^2/F_b^2 = f_e^2/f_b^2 = 1 + (1 - a^2)a^2/d^2. \quad (2b)$$

Furthermore, from the inequality $d^2 \leq (1 - a^2)a^2$ it follows that the n-shell parameter space of our system is a solid cone which we can further restrict as a constant-s disk with coordinates (d, a^2) ([7], Fig. 5). In this disk, systems with a given resonance are represented by constant-d lines; for 1:1 (orthogonal fields) and 1:2 we have $d = 0$ and $d = 3/10$, respectively.

Keplerian or first normal form (average).—The Keplerian or n-shell approximation to the system with Hamiltonian H_{3D} is a 2 degree of freedom Hamiltonian system. For any given $n > 0$, it is defined in terms of dynamical variables $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{y} = (y_1, y_2, y_3)$, which are appropriately rotated [7] combinations of the angular momentum and the eccentricity (also known as Laplace-Runge-Lenz) vectors and which satisfy $\|\mathbf{x}\| = \|\mathbf{y}\| = n/2$. The last relation defines the four-dimensional phase space $\mathbb{S}^2 \times \mathbb{S}^2$. The Poisson algebra generated by the six components of $(\mathbf{x}, \mathbf{y})$ has the standard structure of $so(3) \times so(3)$: $\{x_i, x_j\} = \varepsilon_{ijk}x_k$, $\{y_i, y_j\} = \varepsilon_{ijk}y_k$, and $\{x_i, y_j\} = 0$. The n-shell Hamiltonian on $\mathbb{S}^2 \times \mathbb{S}^2$

$$\Delta E(\mathbf{x}, \mathbf{y}) = \Delta E^{(1)} + \Delta E^{(2)} + \cdots = 2n^2 E - 1,$$

is obtained, following previous work [7,8,11,12], through Kustaanheimo-Stiefel (KS) regularization of H_{3D} and an additional calculation to recover ΔE from the normalized KS Hamiltonian.

Resonances.—ΔE has 2 degrees of freedom and should be normalized further. We turn to the principal (first) order term of ΔE [7]

$$\Delta E^{(1)} = \omega_- x_1 + \omega_+ y_1, \quad (3a)$$

with two frequencies

$$\omega_\pm = \sqrt{(g \pm f_b)^2 + f_e^2} = s\sqrt{1 \pm 2d}. \quad (3b)$$

On $\mathbb{S}^2 \times \mathbb{S}^2$, $\Delta E^{(1)}$ defines a linear Hamiltonian flow, which is a rotation of the two spheres around the axes x_1 and y_1 with respective frequencies ω_- and ω_+. We can normalize a second time with respect to this flow. If $\omega_\pm$ are in resonance (this flow is periodic), we have an $\mathbb{S}^1$ symmetry and we need a resonance specific approach. The same is true near the resonance, i.e., within the corresponding resonance zone.

1:2 *system.*—Here we study the exact resonance $\omega_+ = 2\omega_-$, i.e., $d = 3/10$. We begin with describing all 1:2 systems. Introducing two Hamiltonian functions $\mu = x_1 + 2y_1$ and $\nu = x_1 - 2y_1$, called momenta or actions because they define periodic Hamiltonian $\mathbb{S}^1$ flows on $\mathbb{S}^2 \times \mathbb{S}^2$, we obtain $\Delta E^{(1)} = \omega_- \mu$. The momentum μ defines a dynamical symmetry $\mathbb{S}^1_\mu$ and is central to our analysis. $\mathbb{S}^1_\mu$ acts diagonally on the factors of $\mathbb{S}^2 \times \mathbb{S}^2$ by rotating one of them twice as fast as the other about their respective axes y_1 and x_1 (cf. the recent study [13] of such symmetries).

We normalize and reduce this symmetry using essentially the same universal approach of Ref. [8]. The 1:2 resonant normalized Hamiltonian is expressed in terms of the dynamical variables, $N = \frac{1}{2}(\mathbf{x}^2 + \mathbf{y}^2)$, μ, ν, and the two 1:2 specific cubic polynomials $\pi_1 = \mathrm{Re}\theta$, $\pi_2 = \mathrm{Im}\theta$ with $\theta = 2^3(x_2 + ix_3)^2(y_2 - iy_3)$. It follows that—unlike in the 1:1 systems where the second-order theory typically sufficed—we must, and we do, normalize at least to the third order, the lowest order in which $\pi_{1,2}$ appear. The resulting energy approximation $\Delta\mathcal{E}$ Poisson commutes (to order 3 in our case) with μ and by default,—with N, and can be expressed in terms of the above invariants. Furthermore, due to an additional reversal symmetry $\pi_2 \mapsto -\pi_2$, $\Delta\mathcal{E}$ is a polynomial in (N, μ, ν, π_1) only. Replacing N and μ for their conserved values n and m, which become dynamical parameters, $\Delta\mathcal{E}$ becomes

$$\Delta\mathcal{E}_{n,m}(\nu, \pi_1) = \Delta\mathcal{E}^{\mathrm{scalar}}_{n,m} + \mathcal{H}_{n,m}(\nu, \pi_1), \quad (4a)$$

with $\Delta\mathcal{E}^{\mathrm{scalar}}_{n,m} = \omega_- m + \cdots$ which is independent of dynamical variables (ν, π_1), and the essential part

$$\mathcal{H}_{n,m} = s^2\mathcal{H}^{(2)} + s^3\mathcal{H}^{(3)} + \cdots, \quad (4b)$$

where $\mathcal{H}^{(3)}$ includes the specific 1:2 resonance variable π_1 [14]. Thus we have expressed the original system as a Hamiltonian system with three dynamical variables (ν, π_1, π_2). These variables obey the relation

$$[n^2 - (\mu - \nu)^2/4][n^2 - (\mu + \nu)^2]^2 = \pi_1^2 + \pi_2^2, \quad (5a)$$

and their values are further restricted by the inequalities

$$n \geq 0, \qquad |m + \nu| \leq n, \quad \text{and} \quad |m - \nu| \leq 2n. \quad (5b)$$

We can see that $|m|$ and $|\nu|$ can be only less than or equal to $m_0 = 3n/2$, and that $|\nu|$ reaches m_0 when $|m| = m_1 = n/2$. The relations (5) define a 2D surface $P^{1:2}_{n,m}$ in the 3D

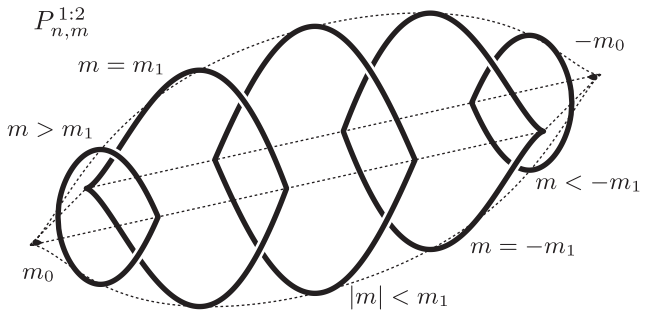

FIG. 1. Intersections (thick black lines) with $\{\pi_2 = 0\}$ of the second reduced phase spaces $P^{1:2}_{n,m}$ of the 1:2 resonant systems. We show intersections for seven different values of m starting at $m = m_0$ and ending at $m = -m_0$. Each such intersection lies on a plane with coordinates (ν, π_1).

space (ν, π_1, π_2) that we call the reduced phase space. The spaces $P^{1:2}_{n,m}$ (see Fig. 1) are spheres with two isolated singular points when $|m| \leq m_1$ and one such point when $m_1 < |m| < m_0$. They are points when $|m| = m_0$.

Energy-momentum map, fibers.—The bifurcation diagram of the energy-momentum map $\mathcal{EM}$ can be constructed by analyzing $\Delta\mathcal{E}_{n,m} = \Delta\mathcal{E}^{\text{scalar}}_{n,m} + \mathcal{H}_{n,m}$ as a function on $P^{1:2}_{n,m}$. Thus the type of the fiber $\{N = n, \mu = m, E = e\}$ can be determined by studying the intersections of the constant-h level sets $\{\mathcal{H}_{n,m}(\nu, \pi_1) = h\}$ with $P^{1:2}_{n,m}$ in the space (ν, π_1, π_2), where $2n^2e - 1 = \Delta\mathcal{E}^{\text{scalar}}_{n,m} + h$.

Connected components of these intersections and the corresponding connected components of the fibers in the initial phase space $\mathbb{R}^6$ will be denoted $\lambda_{n,m,e}$ and $\Lambda_{n,m,e}$, respectively. Any set $\Lambda_{n,m,e}$ that corresponds to an equilibrium in the reduced space, i.e., for which $\lambda_{n,m,e}$ is a single point, is called relative equilibrium (RE). Typically $\lambda_{n,m,e}$ is a smooth circle and $\Lambda_{n,m,e}$ is a smooth $\mathbb{T}^3$. The analysis of the nontypical (critical) intersections gives the following types for $\lambda_{n,m,e}$, its preimage on $\mathbb{S}^2 \times \mathbb{S}^2$, and finally for $\Lambda_{n,m,e}$.

$\Lambda \subset \mathbb{R}^6$	On $\mathbb{S}^2 \times \mathbb{S}^2$	$\lambda \subset P_{n,m}$
$\mathbb{S}^1$ RE	Point	Point space $m = \pm m_0$, $\nu = 0$
$\mathbb{S}^1$ RE	Point	Cuspy point $-\nu = m = \pm m_1$
Short $\mathbb{T}^2$ RE	Short $\mathbb{S}^1$ RE	Any other singular point c
$\mathbb{T}^2$ RE	$\mathbb{S}^1$ RE	Regular point
$\mathbb{S}^1 \times \text{curl}\mathbb{T}^2$	$\text{curl}\mathbb{T}^2$	Singular $S^1 \ni c$
$\mathbb{S}^1 \times \text{bi}\mathbb{T}^2$	$\text{bi}\mathbb{T}^2$	Figure eight
Regular $\mathbb{T}^3$	Regular $\mathbb{T}^2$	Regular $\mathbb{S}^1$

Among the critical components Λ of the $\mathcal{EM}$ map fibers, we recognize the usual four $\mathbb{S}^1$ RE known as Keplerian ellipses [8,12], $\mathbb{T}^2$ RE, and bitori $\text{bi}\mathbb{T}^2$ [8] that appear also in the 1:1 zone. The important 1:2 specific components are short REs and curled tori $\text{curl}\mathbb{T}^2$ [15,16]. Short REs are circular orbits in $\mathbb{S}^2 \times \mathbb{S}^2$ of the $\mathbb{S}^1_\mu$ action with period π instead of 2π. A curled torus consists of an unstable short RE together with its stable and unstable manifolds; see Fig. 2 for a representation.

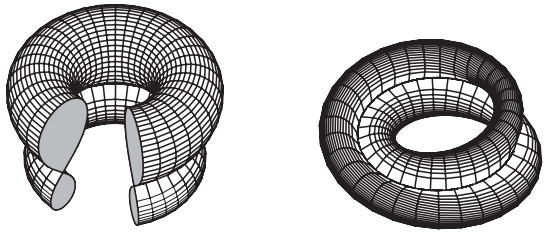

FIG. 2. Bitorus $\text{bi}\mathbb{T}^2$ (left) and curled torus $\text{curl}\mathbb{T}^2$ (right).

Stratified range of $\mathcal{EM}$.—We now turn to the study of a particular 1:2 system with $a^2 = 1/2$ (and $\alpha \approx 0.3\pi$). This system is structurally stable within a large interval of a^2 including those with larger a^2 (smaller α). Furthermore this system is typical of most 1:2 resonant systems.

The set R_n of regular values of $\mathcal{EM}$ for a fixed value of n consists of three parts which we call left and right "legs" and "top" (see Fig. 3). Each leg is attached to the top

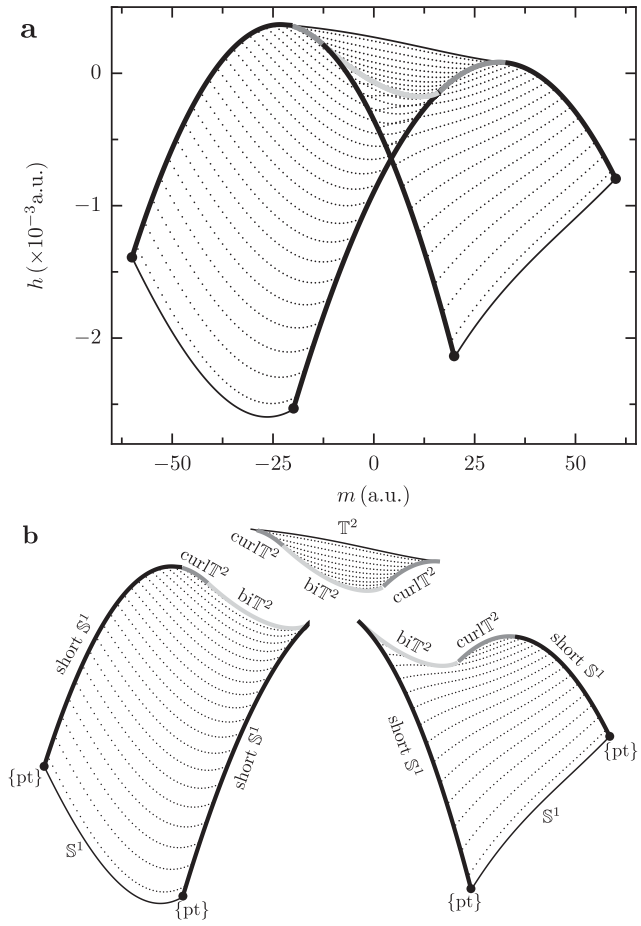

FIG. 3. (a) Joint energy-momentum spectrum (lattice dots) and classical energy-momentum bifurcation diagram (lines) of the 1:2 resonant system with $s = 1/200$, $a^2 = 0.5$, and $d = 0.3$ for $n = 40$ and $\hbar = 1$. (b) Decomposition of the bifurcation diagram in which the three regions have been separated for clarity and where we indicate the type of the fiber in $\mathbb{S}^2 \times \mathbb{S}^2$ along the boundary of each region.

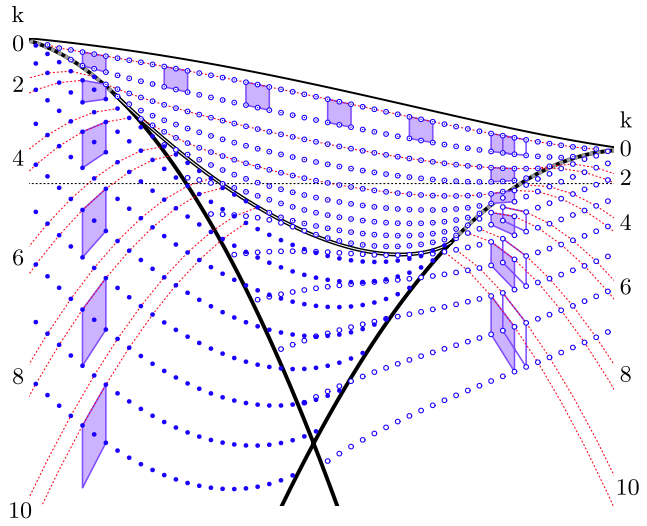

FIG. 4 (color online). Detail of the bifurcation diagram. Dashed lines join states with the same value of the global quantum number k defined by the parallel transport of the elementary cell; below the curl$\mathbb{T}^2$ wall these lines branch in two.

along the respective left and right curl$\mathbb{T}^2$ wall (thick dark gray line) and along the common bi$\mathbb{T}^2$ wall (thick light gray line) in the center, where all three are joined together. Below the bi$\mathbb{T}^2$ wall, the legs overlap necessarily forming a ''flap'' over which each regular fiber has two components.

Joint spectrum.—The system on $\mathbb{S}^2 \times \mathbb{S}^2$ with Hamiltonian $\mathcal{H}_{n,m}$ is quantized by replacing $\mathbf{x}$ and $\mathbf{y}$ for their quantum analogues, and the joint spectrum of commuting quantum operators $(\hat{N}, \hat{\mu}, \hat{\mathcal{H}})$ is computed straightforwardly in the n-shell basis. This spectrum gives a second normal form approximation to that of the initial system with good quantum numbers n and m. In Figs. 3(a) and 3(b), dots within R_n mark quantum states. We see in Fig. 3(b) that in each of the three parts of R_n, the spectrum forms a regular $\mathbb{Z}^2$ lattice. The left and right lattices overlap inside the flap area.

Generalized global action.—The passable curl$\mathbb{T}^2$ walls allow us to relate the $\mathbb{Z}^2$ lattices in each part of R_n thus defining a third global good quantum number k. This is done as follows (Fig. 4). Starting in the top part, we define k locally using a double elementary cell. We transport the cell easily left and right and then bring it down across the curl$\mathbb{T}^2$ walls. Note that the latter operation is possible only for a double cell [15]. At each step we extend the definition of k until every quantum state is reached. The classical analogue of this procedure connects coordinate systems on all regular tori and defines the third global generalized action.

Conclusion and perspectives.—We gave a complete description of the most typical, exactly 1:2 resonant perturbation of the hydrogen atom. We expect that spectroscopy will produce the typical described structure of the energy spectrum for field configurations that give 1:2 resonance, i.e., for angle $\alpha \approx 60°$ between the two fields. Comparing to Ref. [2], which began the study of the 1:1 systems, we would like this Letter to initiate a comprehensive analysis of the rest of the parameter space of this fundamental atomic system.

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