Collapse of the Zeeman structure of the hydrogen atom in external electric field

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Transition from Zeeman to Stark structure in weakly split Rydberg n-multiplet of H atom in parallel magnetic and electric fields is analysed. Classical mechanics together with topological and group theoretical arguments enable us to describe in details the modifications of dynamics under the variation of electric field near the point where the collapse of magnetic Zeeman structure is observed. Sequence of classical bifurcations responsible for the transition between different dynamic regimes is given. Comparison with quantum picture is done.

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Rydberg atoms in parallel magnetic and electric fields have been extensively studied both theoretically and experimentally during the last decade. In particular, many studies have focused on the situation where the fields are (relatively) weak and the dynamics can be analyzed in terms of additional approximate integrals of motion [1–8]. We use a similar idea to analyze several dynamic regimes that exist for different strength of the electric (F) and magnetic (G) fields. These regimes clearly manifest themselves in the energy level pattern in Fig. 1. At very weak electric field, where most of the studies [1–8] have been done, we have a structure characteristic to the second-order Zeeman effect. When F increases this structure quickly disappears. Instead we observe regular "resonance" structures at certain values of F (see Fig. 1). This culminates in an almost complete collapse of the internal structure. Surprisingly, and contrary to the $F \sim 0$ case the dynamics near this collapse has not, to our knowledge, been analyzed. In this paper we give a detailed analysis of the dynamics near the collapse and relate this dynamics to other regimes on the basis of a unified description.

Neglecting the spin effects the Hamiltonian for the hydrogen atom in constant parallel magnetic γ and electric f fields (along the z axis) has the form (in atomic units)

$$H = \frac{p^2}{2} - \frac{1}{r} + \frac{\gamma}{2}L_z + \frac{\gamma^2}{8}(x^2+y^2) - fz, \qquad (1)$$

with γ and f are measured respectively in units of 2.35×10^5 T and 5.14×10^9 V/cm. Several different dynamic regimes are present depending on f and γ values. They clearly manifest themselves through the energy level pattern shown in Fig. 1. In our treatment we restrict ourselves to the low field case when the splitting of n shell caused by both fields is small compared to inter n- gap (see Fig. 3). It is well known that in the absence of electric field m-submanifolds of the n-shell with sufficiently low m show characteristic pattern (second order Zeeman effect) which is destroyed by weak parallel electric field resulting in transition from second order Zeeman structure to Stark structure for separate m submanifold [4,6]. This effect takes place when the electric field effect is of the order of the second order Zeeman effect (see Fig. 2). Up to our knowledge much less attention was paid to the region where the Stark splitting of n shell ($\propto 3fn^2$) becomes of the same order as n shell splitting due to magnetic field ($\propto \gamma n$). (See Fig. 1, region around $3nf/\gamma \approx 1$.) The corresponding relation (collapse condition) for n-shell is

$$f_0 = \gamma/(3n). \qquad (2)$$

To insure that this region corresponds to small n-shell

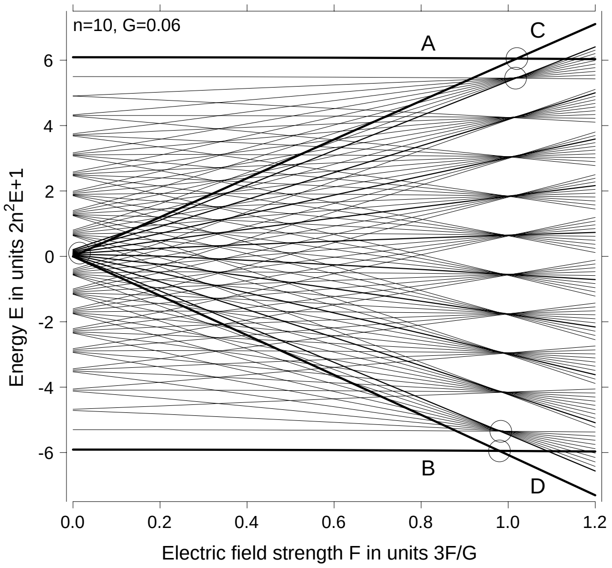

FIG. 1. Collapse of the Zeeman structure for the magnetic field $G = 0.06$ due to the increasing electric field. Quantum levels are calculated for the $n = 10$ multiplet of the hydrogen atom. Electric field strength is given in unit $F_0 = G/3$.

splitting as compared to inter n gap we should take $\gamma < 1/n^4$. Under this assumption we can restrict to the study of isolated n-shell and in such a case it is useful to apply scaling

$$F = fn^4, \quad G = \gamma n^3, \quad \tilde{E}_n = 2n^2 E_n + 1 \tag{3}$$

transforming initial collapse condition (2) into $F_0 = G/3$ and removing n from the effective Hamiltonian (see below Eq. 7).

Our purpose is to study the dynamics under the variation of electric field f in the neighborhood of its critical value f_0. Natural parameter for this deviation is $\delta = 3F/G - 1 = 3fn/\gamma - 1$

The analysis is based on the transformation of the initial Hamiltonian (1) into an effective one for individual n-shell. This can be done by quantum perturbation theory or by classical mechanics by introducing new action angle variables [8,6,7].

An effective quantum Hamiltonian for n-shell and corresponding classical energy function can be expressed in terms of angular momentum $\mathbf{L}$ and Runge-Lenz $\mathbf{A}$ vectors ($\mathbf{A} = \mathbf{p} \times \mathbf{L} - \mathbf{r}/r$), or alternatively in terms of their linear combinations $(J_1)_\alpha = (L_\alpha + A_\alpha)/2$ and $(J_2)_\alpha = (J_\alpha - A_\alpha)/2$. Taking into account only linear in F and G corrections (linear Zeeman and linear Stark effects in parallel fields) the imposed relation between field strengths (2) results in effective Hamiltonian of the form

$$\begin{aligned} H &= \frac{1}{2n^2}(-1 + \gamma n^2 L_z + 3fn^3 A_z) \\ &= \frac{1}{2n^2}(-1 + 3f_0 n^3 (J_1)_z) \end{aligned} \tag{4}$$

which shows clearly that n^2 energy levels in n-shell are groupped in n n-fold degenerate groups with levels in each group labeled by one z-projection of $\mathbf{J}_1$ and different z-projection of $\mathbf{J}_2$. We call this effect the collapse of the Zeeman structure caused by electric field. Quantum energy levels for one n-shell as function of varying electric field are shown in Fig. 1. Second order effects should be taken into account to describe the fine structure of each $(J_1)_z$ manifold of states.

To perform such an analysis the classical description of n-shell hamiltonian function in terms of two pairs of canonically conjugated action-angle variables can be done (see for example [7]). The z-projections of angular momentum and of Runge-Lenz vector can be used as actions. As soon as z-projection of angular momentum is a strict integral of motion the hamiltonian function does not depend on corresponding angle and the only angle conjugated to z-projection of Runge-Lenz vector is present in the hamiltonian function. Instead of direct use of action-angle variables we prefer to use another set of variables to describe both the classical phase space for the effective n-shell problem and the hamiltonian function. The choice of variables is based on group theory and

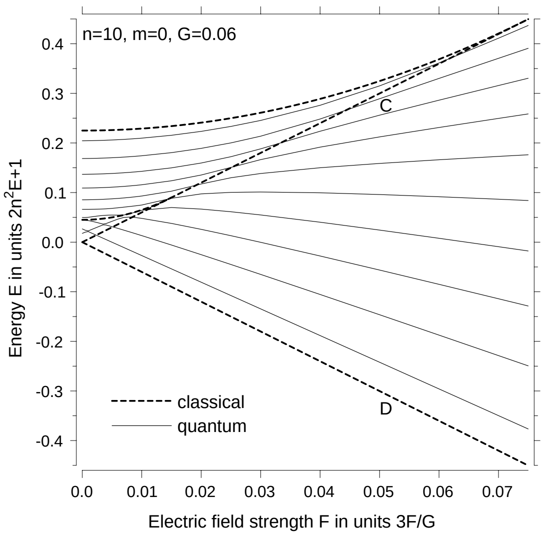

FIG. 2. Deformation of the QZE structure of the $n = 10$, $m = 0$ multiplet of the hydrogen atom. Dashed lines show the energy in stationary points of classical Hamiltonian restricted on $\mu = 0$.

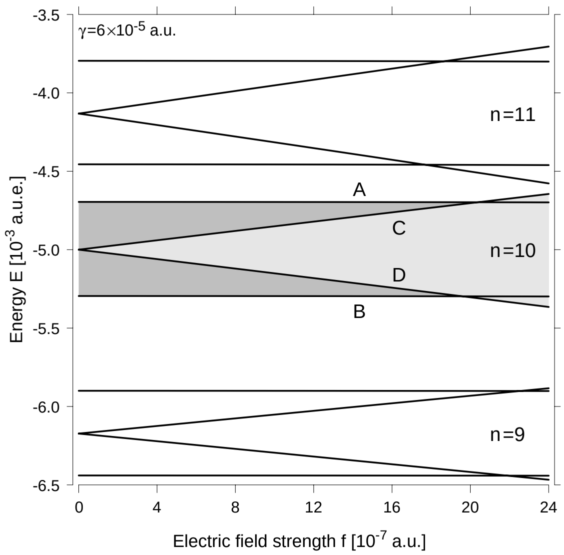

FIG. 3. Neighboring Rydberg multiplets $n = 9, 10, 11$ of the hydrogen atom.

in particular on invariant theory and consist in taking a set of invariant polynomials (forming the so called Integrity Basis) which are used to both labeling the points of the phase space and to expand the hamiltonian function [9–11]. Proper scaling of variables enables us to get equations which do not depend on n.

Symmetry group $\mathcal{G}$ of the problem is generated by the geometrical point group C_∞ and an operation R which is a product of time reversal and a reflection through any plane containing the axis oz (we emphasize that each one of these two perations is not separatly a symmetry of the problem). Remark that R^2 is the identity and the full

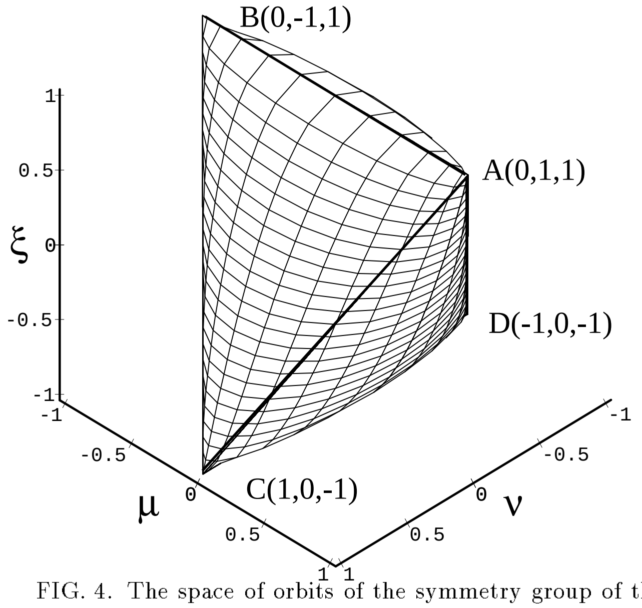

FIG. 4. The space of orbits of the symmetry group of the Rydberg electron in the presence of parallel electric and magnetic fields in the n-shell approximation.

symmetry group $\mathcal{G}$ is isomorphic to $C_{\infty h}$ (but distinct from it).

The classical phase space Σ for effective n-shell hamiltonian is a 4-D space. Its topology is $S_2 \times S_2$ (S_2 is a 2D sphere). The parametrization can be done eigher in L, K variables imposing $J^2 + K^2 = n^2, J \cdot K = 0$, or in J_1, J_2 variables by imposing $J_1^2 = J_2^2 = n^2/4$. (Remark that in classical limit (n is sufficiently large) we neglect 1 as compared to n^2.

The action of symmetry group $\mathcal{G}$ on Σ shows the presence of three types of orbits: 4 critical orbits A, B, C, D which are both C_∞ and R invariant (these 4 orbits are isolated points in Σ); the union of orbits whose point stabilizers are an operation R (each orbit is a S_1 circle); the union of generic orbits (each orbit is formed of two S_1 circles). According to general statement of the invariant theory the system of orbits can be unumbigously characterized by values of invariant polynomials. In the action of $\mathcal{G}$ on Σ every invariant function is made from the three algebraically invariant polynomials, μ, ν, ξ

$$\mu = L_z/n; \quad \nu = A_z/n; \quad \xi = (L^2 - A^2)/n^2. \tag{5}$$

The space of orbits is the orbifold (see Fig. 4) defined by:

$$-1 \leq \xi \leq 1; \quad \sigma = 1 - \xi^2 - 2(1-\xi)\mu^2 - 2(1+\xi)\nu^2 \geq 0. \tag{6}$$

The interior represent the generic orbits. The boundary $\mathcal{B}$ given by equation $\sigma = 0$ represent the other orbits. It is important to note that it contains the edges of the tetrahedron of vertices A, B, C, D. For more details, see Ref. [11].

The hamiltonian function can be equally expressed as a polynomial $H = H(\mu, \nu, \xi)$ of invariant polynomials μ, ν, ξ. Moreover due to invariance with respect to R transformation the hamiltonian does not depend on σ. Up to quadratic in F and G terms the scaled energy $\tilde{E}$ has the form

$$\tilde{E} = G\mu + 3F\nu - \frac{1}{4}G^2\xi + \frac{1}{8}(9F^2 + G^2)\mu^2 + \frac{1}{8}(3F^2 - 5G^2)\nu^2 + \frac{1}{8}(3G^2 - 17F^2) \tag{7}$$

To characterize qualitatively classical and quantum dynamics it is necessary to find the system of stationary points (manifolds) of the energy function on the phase space. Group theory tells us that four points A, B, C, D (critical orbits) are stationary for any smooth function defined over the phase space [9]. Energy values at these points are shown in Figs. 1,3. Morse inequalities confirme that the simplest Morse-type functions possessing stationary points only on the four critical orbits really exist on Σ and have one minimum, one maximum, and two saddle points. For more complicated functions any other stationary points can be found by looking for those energy sections of orbifold which correspond to the modification of the topology of the energy section.

Simple geometrical analysis shows that in the linear (in F and G) approximation for $F < F_0$ the energy function is of the simplest type with minimum in B, maximum in A, and two saddle points in C and D. For $F > F_0$ the energy function is again of the simplest type with minimum in D, maximum in C, and two saddle points in A and B. Sudden transition from one simplest type of the energy function to another in the linear model occurs due to formation of the degenerate stationary manifold for $F = F_0$ value corresponding to Hamiltonian (4). In the linear model the energy surface touches the orbifold through the whole interval $[C, A]$. Introduction of the higher order (in F and G) terms into energy function removes this degenerate case. The energy surface (7) is the second order surface in ξ, μ, ν variables and it can touch orbifold at some points on the $\sigma = 0$ surface different from critical orbits. This means the appearance of additional stationary manifold (in addition to the four critical orbits). The detailed analysis of a system of stationary points as a function of F when F is varying around its collaps value F_0 shows how the transformation from Zeeman type energy function (with only four stationary critical orbits having minimum and maximum in B and A) to Stark type energy function (with only four stationary critical orbits having minimum and maximum in D and C) occurs. Two sequence of bifurcations are present each including two bifurcations. One sequence includes bifurcation at point B which creates new stationary S_1 orbit corresponding to the point on the surface of orbifold which move from B to D and disappears at D after the second bifurcation. Another sequence of bifurcations is similar but now two bifurcations are at C and A and new additional stationary orbit moves from C to A under

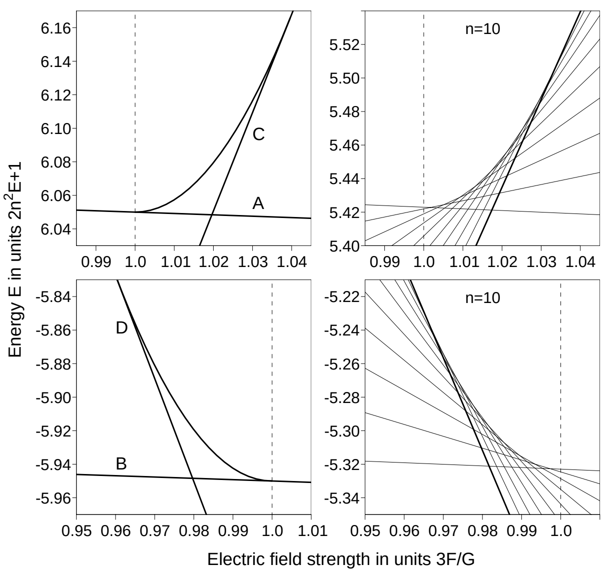

FIG. 5. Bifurcation diagram near the collapse region.

increasing F.

Positions of all stationary orbits can be found by resolving the hamiltonian equation in action angle variables. Alternative way is to use the geometrical representation of orbifold and of the energy surface. Critical orbits are given by symmetry and independent on the concrete form of the hamiltonian. To find noncritical orbits it is necessary to find points where the energy surface touches the orbifold. The corresponding condition is the proportionality of two 3-vectors defined at the same point of the ξ, μ, ν space on the surface $\sigma = 0$. One of these vectors is the normal vector to the $\sigma = 0$ surface and another one is the normal vector to the energy surface. This geometrical view enables us to give extremely simple condition for bifurcations at point A, B, C, D.

$$\text{point } A: \; 4ab = g^2 - b^2; \; \delta_A \approx -G^2/8 - G^3/16 \tag{8}$$

$$\text{point } C: \; 4ag = g^2 - b^2; \; \delta_C \approx 2G/3 + G^2/72 \tag{9}$$

$$\text{point } B: \; 4ab = b^2 - g^2; \; \delta_B \approx -G^2/8 + G^3/16 \tag{10}$$

$$\text{point } D: \; 4ag = b^2 - g^2; \; \delta_D \approx -2G/3 + G^2/72 \tag{11}$$

where a, b, g are correspondingly k_ξ, k_μ, k_ν components of the normal vector $\mathbf{k}$ to the energy surface at point ξ, μ, ν. When δ varies between δ_A and δ_C an additional stationary orbits exits on the surface of the orbifold and moves from the point A to the point C. Similarly for δ between δ_D and δ_B an additional stationary orbits moves from D to B. The energies of all stationary orbits near the bifurcation points together with quantum energy levels are shown in Fig. 5.

Simple physical interpretation of the effect of transformation of the Zeeman type structure into the Stark type one in quantum mechanics can be done by looking at the two extremal states (with minimal and maximal energy) within one n multiplet. We can characterize each extremal state by two average values $< L_z >$ and $< A_z >$. From the positions of stationary points on the orbifold it follows immediately that for the state with maximal energy $< L_z >$ is constant for $\delta < \delta_A$ (and equals the highest possible value), $< L_z >$ is also constant for $\delta > \delta_C$ (and equals zero), whereas for $\delta_A < \delta < \delta_C$ $< L_z >$ varyes almost linearly with δ. For the same state $< A_z >$ is constant for $\delta < \delta_A$ (and equals zero), is constant for $\delta > \delta_C$ (and equals the highest possible value), whereas for $\delta_A < \delta < \delta_C$ $< A_z >$ varyes almost linearly with δ.

With this letter we want to attract the attention to the experimental investigations of the collapse region where important qualitative modifications of dynamics take place. Another object is to demonstrate powerful geometrical and group theoretical technique based on the orbifold representation which is applicable to much wider class of problems related with Rydberg states and which will be presented in details in forthcoming publications [11].

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