Tuning the hydrogen atom in crossed fields between the Zeeman and Stark limits

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We consider the hydrogen atom in the orthogonal electric and magnetic fields whose strength is assumed to be small enough for the Coulomb n-shell perturbation theory to apply. Appropriate scaling of the two fields leads to a uniform parameterization of the problem by S, the combined strength of the two fields, and α, the ratio of the two field strengths. The initial six dimensional phase space R_6 is lifted to the standard Kustaanheimo-Stiefel 8-space and then reduced explicitly to the $S_2 \times S_2$ reduced space of the n-shell using the Lie transformation to the 3-rd order in S. At fixed S the system is uniformly tuned between the Zeeman and the Stark limits using the analytic formulae of the perturbation theory. The approach requires application of the invariant theory, group theory and topology to analysis of the dynamics on the reduced space $S_2 \times S_2$, and subsequent explicit transition to the original R_6. In particular we follow the evolution of the four principal periodic orbits (nonlinear normal modes) and corresponding four relative equilibria on $S_2 \times S_2$.

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I. INTRODUCTION

Hydrogen atom in the presence of static external fields is a fundamental dynamical system with three degrees of freedom. This relatively simple system exhibits many different kinds of dynamical behavior depending on the absolute and relative strengths and on the orientation of the two fields. Thus, the problem of "atoms in fields" has become a test ground for the theoretical methods of the analysis of dynamical systems and of the quantum-classical correspondence. At the same time modern experimental techniques provide highly accurate detailed information on these quantum systems.

In our related paper [1] we develop the orbifold technique to give a concise geometric and dynamical classification for the whole class of problems of atoms in fields. It continues our strategy to apply the methods of nonlinear dynamics, topology, and group theory in concrete problems of atomic and molecular physics [2–4], and we suggest it as a guide.

In the present paper we focus on the hydrogen atom in orthogonal (crossed) electric and magnetic fields [5]. (See Sec. I A for precise definition and notation.) The dynamics of this system can be very complex and it is natural to begin with the nearly integrable case, i.e., at relatively small fields, and to study how the dynamical structure of this case evolves with increasing perturbation.

The main object of our present study is the four families of principal periodic orbits, the nonlinear normal modes, of the crossed field problem, and the corresponding relative equilibria. In this regard we should pay tribute to the two earlier papers, by Flöthmann *et al* [6] and by the group of Uzer and Farrelly [7,8]. In Ref. [6] authors initiate the study of the nonlinear normal modes, which they call "principal Kepler ellipses", in terms of both periodic orbits and adiabatic invariants; the authors of Refs. [7,8] rely essentially on the second order perturbation theory and the dynamical analysis of the reduced Hamilton function of the problem.

The unperturbed hydrogen atom is an integrable system; its three integrals of motion are the orbital momentum L, its projection L_z, and the length of the Runge-Lentz-Laplace vector K. The vectors $\mathbf{L}$ and $\mathbf{K}$ are such that

$$K^2 + L^2 = n^2, \quad (\mathbf{K} \cdot \mathbf{L}) = 0 \ , \tag{1}$$

and the energy is a function of n, $E = -(2n)^{-1/2}$. We consider n, the principal Coulomb integral of motion, as an approximate integral of motion of the atoms-in-fields problems. The quantum analog of n is, of course, the principal quantum number n. This so-called n-shell model is further explained in Sec. II C.

Instead of analyzing the dynamics of our problem directly on the initial six-dimensional phase space R_6, we first use approximate integrability to reduce R_6 to the space of dimension four Σ_4, analyze the dynamics there, and use the correspondence between the reduced and the initial problems. This central dynamical idea of our present paper is explained in Sec. I B.

A. Hydrogen atom in crossed fields

Below we introduce the notation, the Hamilton function, and the symmetry group of our problem. We also define the parameterization which allows a uniform representation of all possible orthogonal field configurations and a convenient "tuning" between the Zeeman and the Stark limit [9].

1. The Hamilton function

The Hamilton function of the hydrogen atom in the presence of constant magnetic and electric fields [10] is

$$H = \frac{P^2}{2} - \frac{1}{r} + (\mathbf{F}\cdot\mathbf{r}) + \frac{1}{2}(\mathbf{G}\cdot\mathbf{L}) + \frac{1}{8}(\mathbf{G}\times\mathbf{r})^2, \quad (2)$$

with $\mathbf{G}$ and $\mathbf{F}$ the magnetic and electric field vectors [11].

To define the coordinate system for the orthogonal (crossed) fields we use the three unit vectors $(\mathbf{n}_b, \mathbf{n}_e, \mathbf{n}_p)$, with $\mathbf{n}_p = \mathbf{n}_b \times \mathbf{n}_e$, such that $\mathbf{F} = F\mathbf{n}_e$ and $\mathbf{G} = G\mathbf{n}_b$. Any vector is represented by three components with indices (b, e, p), for instance $\mathbf{r} = (Q_b, Q_e, Q_p)$. The Hamilton function (2) becomes

$$H = \frac{P^2}{2} - \frac{1}{r} + FQ_e + \frac{1}{2}GL_b + \frac{1}{8}G^2(Q_e^2 + Q_p^2). \quad (3)$$

2. The symmetry group

Our Hamilton function (3) is invariant with regard to three nontrivial discrete spatial-temporal symmetry operations R [9]:

- $\sigma^{(ep)}$ reflection in the plane orthogonal to $\mathbf{G}$,
- $T\sigma^{(eb)}$ combination of time reversal, $(q,p) \to (q,-p)$, and reflection in the plane spanned by $\mathbf{G}$ and $\mathbf{F}$,
- TC_2 time reversal and rotation by π around axis $\mathbf{F}$.

Together with identity I these operations form an order-four group G_4, the total symmetry group of the crossed-field problem. The group G_4 has three order-two subgroups $\mathfrak{g}$,

G_4	C_s	$\mathcal{T}_s$	$\mathcal{T}_2$
$\{I, \sigma^{(ep)}, T\sigma^{(eb)}, TC_2\}$	$\{I, \sigma^{(ep)}\}$	$\{I, T\sigma^{(eb)}\}$	$\{I, TC_2\}$

which we will use in the paper.

3. Parameterization

We want to study how the dynamics of the problem depends on the ratio of the field strengths when the total effect of two orthogonal fields is kept more or less the same all the way from the pure Zeeman effect configuration to the pure Stark effect configuration [9,12].

To define this total effect we take into account that the first order (linear) correction ΔE_n to the n-shell energy of the hydrogen atom in the Zeeman and Stark limit is, respectively, $\approx \pm Gn^3$ and $\approx \pm 3Fn^4$ where the value of n, the principal Coulomb integral for the perturbed hydrogen atom, is $\approx \sqrt{-1/(2E)}$. Then for given n it is natural to fix

$$S = \sqrt{(Gn^3)^2 + (3Fn^4)^2}, \quad (4a)$$

and to vary only the relative strengths of the two fields:

$$G_s = Gn^3/S, \quad F_s = 3Fn^4/S. \quad (4b)$$

In this paper we consider small values of S and *all* possible relative strengths of the two fields. The latter can be conveniently represented as

$$F_s = \cos\alpha, \quad G_s = \sin\alpha, \quad 0 \le \alpha \le \frac{\pi}{2}. \quad (4c)$$

B. Correspondence between the reduced and the initial phase spaces

Several limiting physical situations correspond to the complete or partial integrability of the equations of motion defined by the Hamilton function (3). Continuous spatial symmetry O(3) of the unperturbed problem results in the strict integrals of motion L and L_z; The "extra" Coulomb symmetry, also continuous, is associated with the integral K. In the case of the two orthogonal fields these continuous symmetries are broken (Sec. I A 2), and generically this classical system should be analyzed on a six-dimensional phase space.

At the same time we consider the principal Coulomb integral n in Eq. (1) as an *approximate* integral of motion. In fact, this approach is quite typical: in a physical problem with N degrees of freedom and the phase space $R_{2N}(q_1, \ldots, p_N)$, we often can introduce an approximate integral of motion n with conjugate angle ϕ_n and reduce the problem to one with $N-1$ degrees of freedom and the phase space Σ_{2N-2}.

1. The reduction procedure

We can reduce the original Hamilton function H with regard to n if H is (can be represented as) a formal power series at $Q = P = 0$,

$$H(Q,P) = H_0(Q,P) + \sum_{k=1} \frac{\epsilon^k}{k!} H_k(Q,P)\ , \quad (5)$$

whose zero order H_0 is linear in n and depends only on n. We introduce the formal smallness parameter ϵ and classify the orders k of the perturbation theory by the total degree in (Q,P) of the corresponding term H_k. We reduce H by averaging the dynamics of our system with regard to the angle ϕ_n. More precisely, we eliminate all such high-order terms in H_k that $\{H_k, H_0\} \ne 0$ by an appropriate canonical transformation.

The resulting Hamilton function of the reduced problem is called the *normal form* $H_{\text{n.f.}}$, and the perturbation technique generally used for reduction is called the normal form transformation. In this technique we build a canonical near identity change of variables, a Lie transformation $\mathfrak{L}$, that transforms the original phase space R_{2N} into a space of the same dimension (and topology) $\mathcal{R}_{2N}$,

$$R_{2N} \xrightarrow{\mathfrak{L}} \mathcal{R}_{2N} \mapsto \Sigma_{2N-2}. \quad (6)$$

At the same time the normal form $H_{\rm n.f.}$ defined on $\mathcal{R}$ is a function of only $2N-2$ dynamical variables, since the quantity n plays the role of a parameter and the angle ϕ_n is ignorable (the $H_{\rm n.f.}$ does not anymore depend on ϕ_n). Therefore, we can consider $H_{\rm n.f.}$ as a Hamilton function defined on a *reduced* phase space of dimension $2N-2$, and we will call this space Σ.

However, since n is only an approximate integral of motion, $H_{\rm n.f.}$ is obtained as a formal power series and, generally, is divergent. Physically it is clear that we cannot equivalently replace an original nonintegrable system by an integrable one. Nevertheless, we can still understand many important global features of this original system using our divergent $H_{\rm n.f.}$.

Thus, to actually use Σ in the analysis of the dynamics of a concrete problem we assume that n is a strict integral of motion. Technically this occurs when we *truncate* $H_{\rm n.f.}$. The extent to which we can represent the original dynamics clearly depends on how good an approximate integral of motion n is.

2. Reduced phase space Σ

Apart from dimension, the main difference between Σ_{2N-2}, the phase space of the equations of motion defined by the $H_{\rm n.f.}$, and the initial phase space R_{2N} lies in their global properties: while R_{2N} is a simple Euclidean space (with some standard symplectic structure $dq \wedge dp$), the topology of Σ_{2N-2} and the symplectic structure on Σ_{2N-2} depend on the nature of the approximate integral of motion n, i.e., on the approximate dynamical symmetry we assume. They can be quite complex.

The dynamical structure on the reduced phase space Σ_{2N-2} has two aspects, a global aspect and a particular aspect. The former is entirely defined by the topology of Σ and is *not* dependent on the concrete $H_{\rm n.f.}$. In other words, due to the nature of the approximate integral n, the dynamical structure of *any* particular generic reduced problem obtained with this n will have certain common features.

In our case the nucleus is assumed to rest at the origin and the electron moves around in the three dimensional space, i.e., N=3 and the original phase space is R_6. When we introduce n as an approximate integral of motion the four-dimensional reduced phase space becomes $\Sigma_4 = S_2 \times S_2$, the direct product of two two-dimensional spheres (Sec. II C).

3. Dynamical structure on Σ *and on* R

Assuming the integrability in n, the dynamical structure on the reduced space Σ_{2N-2} can be easily lifted to the transformed phase space $\mathcal{R}_{2N}$ by adding a periodic motion with angle ϕ_n. In other words, if we have a dynamically invariant subspace $\Gamma \in \Sigma$ of the reduced space Σ, the image of Γ in $\mathcal{R}$ is simply a product of Γ and a circular orbit S_1 defined by ϕ_n, i.e., $\Gamma \otimes S_1(\phi_n)$. To obtain the image in the original phase space R we use the inverse transformation $\mathfrak{L}^{-1} : \mathcal{R} \to R$ (cf. Eq. 6).

In the simplest case, stationary points on Σ correspond to periodic orbits on R with ϕ_n the natural coordinate along these orbits. Periodic orbits on Σ correspond to invariant two-dimensional tori T_2 in R.

C. Symmetry analysis

The Hamilton function $H(Q,P)$ in Eq. (3) of our problem is invariant with respect to all operations R of the group G_4 introduced in Sec. I A 2. These operations act on the initial phase space $R_{2N}(Q,P)$ with $N=3$ and thus on any function defined on R_{2N}. By construction, our normal form transformation $\mathfrak{L}$ preserves the G_4 symmetry [13] and so $H_{\rm n.f.}$ inherits this symmetry from the initial Hamilton function (3).

To understand the consequences of this symmetry we study the *action* of the operations R of G_4 on the points of, and on the scalar functions on the phase space, as well as on other dynamical objects, such as vector fields, flows, and periodic orbits [14]. As a result the phase space is subdivided into *strata*, or sets of points with different symmetry properties. (We say that the phase space is stratified under the action of the symmetry group [15].) Strata of dimension zero, i.e., sets of isolated points, are of particular interest since they necessarily correspond to the stationary points of any smooth G_4-invariant Hamilton function. We also distinguish invariant subspaces which can be composed of several different strata.

Once the action of the symmetry group $\mathfrak{G}$ on the initial phase space R is given, the relation (6) defines the action of $\mathfrak{G}$ on the reduced phase space Σ. The action of G_4 on the reduced phase space $\Sigma = S_2 \times S_2$ of our problem is analyzed in Appendix A. This action is nontrivial, so that in addition to the topological requirements on the generic Hamilton functions over Σ there are requirements due to symmetry. In particular, the Morse theory gives the lower boundary for the number of stationary points and the constraints on the possible positions and stabilities of these points. In other words, within some domain in the control parameter space, for any generic G_4-invariant Hamilton function $H_{\rm n.f.}$ on Σ there is a minimal set of stationary points (relative equilibria) which with regard to the control parameters forms a continuous parametric set. This set consists of continuous families formed by each stationary point. Each family corresponds to a family of periodic orbits in the original phase space R, called the *nonlinear normal mode*.

1. Spatial symmetry

In the simplest case we deal with *linear symplectic* operations R which are easily applied to any of the above objects. The $\sigma^{(ep)}$ operation,

$$\sigma^{(ep)} : (Q, P) \to (Q_e, -Q_b, Q_p, P_e, -P_b, P_p), \qquad (7)$$

is an example, it is a point transformation of the physical 3D space, the configuration space, and is symplectically extended to the phase space. One of the main consequences of this spatial symmetry is the existence of the dynamically invariant subspace of the phase space R_6. Indeed, equation $Q_b = P_b = 0$ defines the $\sigma^{(ep)}$-invariant four-dimensional subspace of R_6. The $\sigma^{(ep)}$-invariant subspace is also dynamically invariant: any trajectory with initial conditions $Q_b = P_b = 0$ will remain in this subspace, i.e., the electron will move in the plane (ep) orthogonal to the magnetic field vector $\mathbf{G}$. Two major periodic orbits of the entire problem lie in this plane and can, therefore, be studied more easily using the restricted Hamilton function. We consider the C_s-restricted dynamics along with the general off-plane case with three degrees of freedom.

2. Spatial-temporal symmetry

Operations of G_4 which involve time reversal T require slightly different approach. In fact, these operations cannot be adequately represented on the phase space, i.e., using only coordinates and conjugated momenta. Formally their action can still be defined. This action is not symplectic and does not preserve the Hamiltonian flow (does not commute with this flow). Therefore, we should bear in mind that such action can only be useful for the analysis of stationary points.

For example, the action of the $T\sigma^{(eb)}$ operation

$$(Q, P; t) \to (Q_e, Q_b, -Q_p, -P_e, -P_b, P_p; -t), \qquad (8a)$$

on the phase space can be formally given by a non-symplectic operation

$$T\sigma^{(eb)} : (Q, P) \to (Q_e, Q_b, -Q_p, -P_e, -P_b, P_p), \qquad (8b)$$

and as such can be applied to a time-independent Hamilton function (3). The result can be used to find additional constraints on the number, position, and type of stationary points of H in the same way as for any other symmetry operation discussed above. However, the action of (8a) on the Hamiltonian vector field and on the trajectories cannot be deduced from its action on the individual points of the phase space (8b). As a result, except for the singular points, any structure that exists on the phase space due to (8b) is irrelevant to the behavior of the flow of the dynamical system. The role of spatial-temporal symmetries for the hydrogen atom problem is further considered in Sec. III B.

3. Dynamical symmetry with nonlinear action

More complicated are situations where operations R in the total symmetry group $\mathfrak{G}$ have *nonlinear* action on the initial phase space. Our zero order, the Hamilton function H_0 of the unperturbed hydrogen atom, is such example. Its total dynamical symmetry group SO(4) has nonlinear action on the initial phase space R_6. This has important consequences. We consider dynamical symmetry properties of H_0 as approximate symmetries, and we transform our initial Hamilton function to a normal form $H_{\text{n.f.}}$ which, up to a given order in the small perturbation parameter, preserves these dynamical symmetries *exactly*. It follows that, as described later in Sec. II A, the most natural and simple approach is to *linearize* the action of our approximate dynamical group $\mathfrak{G}$ by lifting our initial phase space R_6 up to a space of higher dimension. In this way we can easily combine and analyze all symmetries of the problem.

II. REDUCED PROBLEM FOR CROSSED FIELDS

A. Reduction or enlargement?

From the physical point of view the natural way to simplify the problem consists of taking into account the exact (or approximate) integrals of motion. We consider our integrals as exact and transform the initial Hamiltonian problem into a reduced problem which has fewer variables. More precisely, when we introduce an integral of motion n, we begin to study our system independently (separately) for single individual values of n. Since the conjugated angle ϕ_n is ignorable we consider all points of the initial phase space R that differ only in the value of ϕ_n as *equivalent*. In other words, we regard the change of ϕ_n as an operation of some continuous dynamical symmetry group G. In particular, to find the group orbit of G corresponding to a point (q_0, p_0) of R we can consider the trajectory of the dynamical system with Hamilton function $H = n$ and with initial conditions (q_0, p_0).

Traditionally such procedure is regarded as "simplification" since the number of variables is reduced. (The dimension of the reduced phase space $\dim\Sigma$ is related to the dimension of the initial phase space, $\dim R$, as $\dim\Sigma = \dim R - 2\dim G$, where $\dim G$ is the number of continuous parameters of the dynamical symmetry group G, i.e., the number of independent integrals of motion.) At the same time the Hamiltonian flow on the reduced phase space naturally becomes more complicated and more difficult to handle.

The procedure of the reduction, and especially the correspondence of the points on Σ and R can be easily defined if the action of the dynamical symmetry group G on

R is linear, i.e., G is a group of linear symplectic transformations of R. In many problems, and in particular for the hydrogen atom, this is not the case. The general mathematical statement, the Mostow theorem, assures that the linearization of the group action is possible by *enlargement* of the initial space [16,17]. From the physical point of view this means that it is always possible to consider the real initial physical system with a complicated Hamiltonian flow as a formal result of the reduction of a simpler Hamiltonian flow defined on a phase space of higher dimension.

The initial phase space of the hydrogen atom problem (as well as of the Kepler problem) is R_6 of dimension six. The spatial symmetry of the unperturbed problem is $O(3)$ but the dynamical symmetry group G corresponding to the integral n is higher. Thus our work is based on $G = O(4)$, the orthogonal group in 4-space. To linearize the action of $O(4)$ we enlarge the dimension of R by two. The actual transition $R_6 \to R_8$ is given by the Kustaanheimo-Stiefel (KS) transformation [18,19]. The R_6 is obtained from the KS space R_8 as a space reduced with regard to the auxiliary integral of motion $\zeta(q,p) = 0$ by identifying all points which differ only in the value of the conjugated angle ϕ_ζ.

The second but not least important reason for the KS transformation is the *regularization* of the $1/r$ Coulomb potential of our problem [20]. Indeed, the normal form reduction that we want to apply (Sec. I B 1) works only in problems whose Hamilton function H is regular near the equilibrium $Q = P = 0$ [cf. Eq. (5)]. In the KS coordinates the Hamilton function (3) is regularized simply by taking $H \to Hr$ (so that time becomes $t \to t/r$) and the problem transforms into a four-dimensional oscillator. See the details below.

B. KS transformation and regularization

The KS transformation [Ref. [18], II.9 Eq. (27)] is defined by the matrix

$$M_{\mathrm{KS}} = \begin{pmatrix} q_1 & -q_2 & -q_3 & q_4 \\ q_2 & q_1 & -q_4 & -q_3 \\ q_3 & q_4 & q_1 & q_2 \\ q_4 & -q_3 & q_2 & -q_1 \end{pmatrix}, \tag{9}$$

with $q_1, \ldots, q_4$, the coordinates in R_4. The coordinates (Q_1, Q_2, Q_3) in the three-dimensional physical space are obtained as

$$(Q_1, Q_2, Q_3, Q_4)^T = M_{\mathrm{KS}}\,(q_1, q_2, q_3, q_4)^T, \tag{10a}$$

where M_{KS} is such that $Q_4 \equiv 0$. In particular, the radius in the 3-space equals

$$r = \sqrt{Q_1^2 + Q_2^2 + Q_3^2} = q_1^2 + q_2^2 + q_3^2 + q_4^2\ , \tag{10b}$$

and $M_{\mathrm{KS}}^T M_{\mathrm{KS}} = M_{\mathrm{KS}} M_{\mathrm{KS}}^T = r I_4$. The momenta (P_1, P_2, P_3) of the initial phase space R_6 are expressed in terms of coordinates (q_1, q_2, q_3, q_4) and conjugated momenta (p_1, p_2, p_3, p_4) in R_8 as

$$(P_1, P_2, P_3, P_4)^T = \frac{1}{2r} M_{\mathrm{KS}} (p_1, p_2, p_3, p_4)^T\ , \tag{11a}$$

so that

$$P_1^2 + P_2^2 + P_3^2 + P_4^2 = \frac{1}{4r}(p_1^2 + p_2^2 + p_3^2 + p_4^2)\ , \tag{11b}$$

i.e., the kinetic energy in the KS space R_8 acquires factor $1/r$, the *same* as in the Coulomb potential. The KS transformation defined by Eqs. (10) and (11) is canonical with regard to the conjugated variables (Q_1, P_1), (Q_2, P_2), (Q_3, P_3): the Poisson brackets $\{Q_\alpha, P_\beta\}$ calculated with (q_1, q_2, q_3, q_4) and (p_1, p_2, p_3, p_4) remain the same. However, in order for P_4 in Eqs. (11) become identically zero we impose the restriction

$$\zeta \stackrel{\mathrm{def}}{=} -2rP_4 = q_1 p_4 - q_4 p_1 + q_3 p_2 - q_2 p_3 = 0. \tag{12}$$

Thus the initial phase space $R_6 = \{Q_1, Q_2, Q_3, P_1, P_2, P_3\}$ of the Kepler problem becomes a reduced space for a problem in the $R_8 = \{q_1, q_2, q_3, q_4, p_1, p_2, p_3, p_4\}$ with integral of motion $\zeta = 0$ [21]. Using the KS formulae (10) and (11) together with condition (12) we express the angular (orbital) momentum

$$(L_1, L_2, L_3) = (Q_1, Q_2, Q_3) \times (P_1, P_2, P_3)\ , \tag{13}$$

in the 3-space in terms of R_8:

$$L_b = \tfrac{1}{2}(q_1 p_4 - q_4 p_1 + q_2 p_3 - q_3 p_2) = q_2 p_3 - q_3 p_2, \tag{14a}$$

$$L_e = \tfrac{1}{2}(q_2 p_4 + q_3 p_1 - q_1 p_3 - q_4 p_2), \tag{14b}$$

$$L_p = \tfrac{1}{2}(q_1 p_2 + q_3 p_4 - q_2 p_1 - q_4 p_3), \tag{14c}$$

where for the purpose of this work we use the (e, b, p) notation for the components of vectors in the 3-space introduced in Sec. I [cf. Eq. (3)], i.e., $(1, 2, 3) = (e, b, p)$. Note that the three unit vectors $(\mathbf{n}_b, \mathbf{n}_e, \mathbf{n}_p)$ form a usual right hand frame, and correspondingly the Poisson bracket $\{L_b, L_e\}$ equals L_p. We also note, that ζ together with (L_b, L_e, L_p) realize four of the six generators of the SO(4) group of rotations of the (q_1, q_2, q_3, q_4) space.

1. The Hamilton function in the KS coordinates

We substitute Eqs. (10), (11b), and (14a) into the equation

$$H(P, Q) = E, \tag{15a}$$

with $H(P, Q)$ defined in Eq. (3) and E the energy. Expressed in terms of (q, p), the variables in R_8, Eq. (15a) is regularized by multiplying both sides on $4r$,

$$4rH(p, q) - 4rE = 0. \tag{15b}$$

This new equation is a polynomial in (q, p) whose quadratic part

$$\tfrac{1}{2}p^2 + (-8E)\tfrac{1}{2}q^2 + \ldots = 4, \tag{15c}$$

represents a four-dimensional isotropic harmonic oscillator with frequency

$$\omega = \sqrt{-8E}. \tag{16}$$

Scaled to the standard form by

$$(p, q) \to (p\sqrt{\omega}, q/\sqrt{\omega}), \tag{17}$$

our equation finally becomes

$$\tfrac{1}{2}(p^2+q^2) + \tfrac{1}{3}f(q_2q_1 - q_4q_3)q^2 + \tfrac{1}{2}g(q_2p_3 - q_3p_2)q^2 + \tfrac{1}{8}g^2(q_2^2+q_3^2)(q_1^2+q_4^2)q^2 = \frac{4}{\omega}\ , \tag{18}$$

with auxiliary field parameters

$$g = 4G/\omega^2, \quad f = 24F/\omega^3\ . \tag{19}$$

In the action-angle variables, the harmonic part of the oscillator (18) becomes the total action which should be proportional to the principal integral of motion n of the unperturbed Coulomb problem. Since for the Coulomb problem $4/\omega = 2n$ [cf. Eq. (16)],

$$2n = \tfrac{1}{2}(p_1^2+p_2^2+p_3^2+p_4^2+q_1^2+q_2^2+q_3^2+q_4^2). \tag{20}$$

2. Laplace-Runge-Lentz vector

To find the KS expression for the Laplace-Runge-Lentz vector we begin with its definition in the initial physical space [cf. Eqs. (21) and (22) of Ref. [22] and Ref. [23]],

$$\mathbf{K} = \mathbf{P}\times\mathbf{L} - \mathbf{Q}/r. \tag{21}$$

Substitution of the KS formulae for Q, P, and L in Eqs. (10), (11), and (14) yields complicated expressions which, however, can be radically simplified by taking into account $\zeta = 0$ [Eq. (12)] and using our assumption $n = \text{const}$, i.e., restricting (21) on a sphere S_7 in R_8. The radius of this sphere can be chosen arbitrarily and the value of $4n = 8$ results in the desired simplification. Since this implies $n = 2$, we rescale the result, $K \to 2K$, to obey the standard relations (1) and obtain the KS expressions in their final form,

$$K_b = \tfrac{1}{4}(p_2^2+q_2^2+q_3^2+p_3^2-q_1^2-p_1^2-q_4^2-p_4^2), \tag{22a}$$
$$K_e = \tfrac{1}{2}(p_4p_3 - q_2q_1 - p_1p_2 + q_4q_3), \tag{22b}$$
$$K_p = -\tfrac{1}{2}(q_3q_1 + p_1p_3 + q_4q_2 + p_4p_2). \tag{22c}$$

We can now to verify the usual Poisson brackets

$$\{L_e, L_b\} = L_p, \quad \{L_e, K_b\} = K_p, \quad \{K_e, K_b\} = L_p, \tag{23}$$

using Eqs. (14) and (22). This concludes the hydrogen atom realization of the standard so(4) algebra with generators $(L_e, L_b, L_p, K_e, K_b, K_p)$.

3. Standard diagonal representation

We can greatly accelerate the procedure of the normal form reduction of the Hamilton function (18) by changing to coordinates $(q', p')^T = U^{-1}(q, p)^T$, with U the 8×8 symplectic transformation matrix,

$$U = \begin{pmatrix} 0&0&0&-1&-1&0&0&0\\ 0&1&0&0&0&0&-1&0\\ 0&0&1&0&0&-1&0&0\\ 1&0&0&0&0&0&0&1\\ 1&0&0&0&0&0&0&-1\\ 0&0&1&0&0&1&0&0\\ 0&1&0&0&0&0&1&0\\ 0&0&0&-1&1&0&0&0 \end{pmatrix}\frac{1}{\sqrt{2}}, \tag{24}$$

such that the quadratic form $\zeta(q', p')$ [Eq. (12)] is diagonal [24]. In these new coordinates, four quantities,

$$n = \tfrac{1}{2}(n_1+n_2+n_3+n_4), \tag{25a}$$
$$\zeta = -n_1 - n_2 + n_3 + n_4\ , \tag{25b}$$
$$K_b = \tfrac{1}{2}(-n_1+n_2+n_3-n_4), \tag{25c}$$
$$L_b = \tfrac{1}{2}(-n_1+n_2-n_3+n_4) = n_2 - n_3\ , \tag{25d}$$

have diagonal representation in terms of actions of four one-dimensional oscillators $n_i = \frac{1}{2}({q'}_i^2 + {p'}_i^2)$, $i = 1\ldots 4$.

Due to the invariance of Eq. (18) with respect to the SO(2) rotations generated by ζ, the Hamilton function $H(q', p') = H(q, p)$ as a whole necessarily commutes with ζ, $\{H, \zeta\} = 0$. In other words, ζ is an integral of motion. In the $z_i = {q'}_i \pm i{p'}_i$ coordinates, the operation $\{, \zeta\}$ maps each individual monomial $h = z_1^{a_1}\ldots z_4^{a_4}\bar{z}_1^{b_1}\ldots\bar{z}_4^{b_4}$ onto itself. It follows that all monomials h of H are in the null-space of $\{, \zeta\}$ and every h commutes with ζ. The representation of H in terms of such "ζ-invariant" monomials h requires the minimal number of terms [equal to the dimension of the null-space for each degree $a_1 + \ldots + a_4 + b_1 + \ldots + b_4$]. This in turn minimizes the number of terms in the generator of $\mathfrak{L}$ and hence the memory load and computation time of the reduction procedure [13].

Another important application of the coordinates (24) is the standard algebraic and geometric representation of the problem. These coordinates give an explicit geometric construction of the embedding of the reduced phase space Σ of the problem into the initial R_8 and transformed $\mathcal{R}_8$ KS spaces in terms of angles ϕ_i and conjugated actions n_i of four oscillators. See Secs. II C and IV D and Ref. [7] for further details.

4. Restriction on the C_s-invariant subspace

As already pointed out in Sec. I C 1, the crossed fields problem possesses one purely spatial symmetry $\sigma^{(ep)}$ in Eq. (7) and its spatial symmetry group is C_s.

To study the C_s-invariant dynamics we find the image of $\sigma^{(ep)}$ in the KS space R_8 and the defining equations of the C_s-invariant subspace(s). In fact it suffices to find one realization of $\sigma^{(ep)}$, such as

$$\sigma^{(ep)} : (q_1, q_2, q_3, q_4) \to (q_2, q_1, q_4, q_3), \tag{26a}$$

and one corresponding invariant subspace in R_8 with

$$q_1 = q_2, \quad q_3 = q_4, \quad p_1 = p_2, \quad p_3 = p_4, \tag{26b}$$

[cf. coordinates $Q_\alpha(q_1, q_2, q_3, q_4)$ in Eq. (10) and use Eq. (12) when verifying the invariance of (18)]. All other C_s-invariant subspaces are equivalent and are mapped into the same (Q_e, Q_p, P_e, P_p)-plane of the original phase space R_6.

Restriction of Eq. (18) by relations (26b), results in a two-degrees-of-freedom problem with Hamilton function

$$\tilde{H} = p_2^2 + q_2^2 + p_4^2 + q_4^2 + \frac{2}{3}(q_2^4 - q_4^4)f + (q_2 + q_4)(q_2 p_4 - q_4 p_2)g + \frac{1}{4}(q_2^2 + q_4^2)^3 g^2 = \frac{4}{\omega}. \tag{27}$$

It follows that in the KS coordinates the C_s restricted problem has two degrees of freedom, the same as in the (ep) plane of the initial physical space.

We use Eqs. (26b) to find the restriction of of the principal Coulomb integral n in Eq. (20), of ζ in Eq. (12), as well as of vectors $\mathbf{L}$ in Eq. (14) and $\mathbf{K}$ in Eq. (22). Four of these quantities are not invariant with regard to $\sigma^{(ep)}$ in Eq. (26a) and hence vanish,

$$\tilde{L}_e = \tilde{L}_p = \tilde{K}_b = \tilde{\zeta} \equiv 0, \tag{28}$$

(cf. Table I below). Four others remain quadratic polynomials on $R_4 \in R_8$,

$$\tilde{n} = \tfrac{1}{2}(q_2^2 + p_2^2 + q_4^2 + p_4^2), \tag{29a}$$

$$\tilde{L}_b = q_2 p_4 - q_4 p_2, \tag{29b}$$

$$\tilde{K}_e = \tfrac{1}{2}(q_4^2 + p_4^2 - q_2^2 - p_2^2), \tag{29c}$$

$$\tilde{K}_p = -q_2 q_4 - p_2 p_4. \tag{29d}$$

C. Reduced phase space $S_2 \times S_2$

The KS transformation defines the correspondence between the R_8 phase space and the initial R_6 space as reduction with the exact “integral of motion” $\zeta = 0$. At the same time we consider weakly perturbed hydrogen atom where n, the principal Coulomb integral of motion, is a good approximate integral. Reduction with regard to n is realized in the R_8 space as a standard Lie transformation (6). The four-dimensional reduced space Σ_4 is obtained from the transformed space $\mathcal{R}_8$ using both $n = \text{const}$ and $\zeta = 0$.

Since in the reduced problem the Hamilton function is truncated and n is considered as a strictly conserved quantity, the phase space Σ_4 is the same as for the unperturbed hydrogen atom. We can use the components of the orbital angular momentum L and those of the Runge-Lentz vector K with two restrictions (1) as dynamical coordinates on this space. It is convenient to take advantage of the $n = \text{const}$ condition and introduce universal scaled vectors, such that

$$\mathbf{K} \to \mathbf{K}/n, \quad \mathbf{L} \to \mathbf{L}/n, \quad K^2 + L^2 \to 1 \tag{30a}$$

In other words, we project any given n-shell on the shell $n = 1$. Note that in the transformed space $\mathcal{R}_8$ this means scaling all KS coordinates

$$q \to q/\sqrt{n}, \quad p \to p/\sqrt{n}\ , \tag{30b}$$

i.e., $\sqrt{n}$ plays the role of a hyperradius in $\mathcal{R}_8$.

Alternatively, the six components of the two vectors

$$\mathbf{J}_1 = \tfrac{1}{2}(\mathbf{L} + \mathbf{K}), \quad \mathbf{J}_2 = \tfrac{1}{2}(\mathbf{L} - \mathbf{K}), \tag{31}$$

with two (n-scaled) restrictions

$$\mathbf{J}_1^2 = \mathbf{J}_2^2 = \tfrac{1}{4} = \text{const}, \tag{32}$$

are often used. Since $\{J_{1\alpha}, J_{2\beta}\} = 0$ [cf. Eqs. (23)] we immediately conclude that the phase space Σ_4 is a direct product of two two-dimensional spaces. Furthermore, since each $\mathbf{J}_i$ has the properties of the angular momentum, i.e., $\{J_{ie}, J_{ib}\} = J_{ip}$, and the magnitude of each $\mathbf{J}_i$ is fixed, Σ_4 is a direct product of two two-dimensional spheres, $\Sigma_4 = S_2 \times S_2$.

Due to the $S_2 \times S_2$ topology any generic Hamilton function $H_{\text{n.f.}}$ on Σ_4 must have at least four stationary points, a minimum, a maximum, and two saddle points with Morse index 2. The presence of discrete symmetry results in further necessary special features of $H_{\text{n.f.}}$ discussed below. The topology of Σ also restricts possible deformations of the generic dynamical structure due to the change of control parameters, such as energy, the value of n, etc.

1. Reduced phase space of the C_s restricted problem

The C_s restricted problem (27) is similar to many other problems with two degrees of freedom, such as, for instance, the Hénon-Heiles oscillator. In all these problems reduction is made near the equilibrium $q = 0$ with regard to the combined action of the two harmonic oscillators, such as $\tilde{n}$ in (29). The reduced phase space is a two-sphere S_2 (or the isomorphic complex projective space CP_1), which in our case is a C_s-invariant subspace of the reduced space Σ (Sec. III A).

The coordinates $(\tilde{L}_b, \tilde{K}_e, \tilde{K}_p)$ on this sphere are already defined in Eq. (29). Indeed, after normalization (30a)

$$\tilde{L}_b^2 + \tilde{K}_e^2 + \tilde{K}_p^2 = 1. \tag{33}$$

In fact, expressions for $(\tilde{L}_b, \tilde{K}_e, \tilde{K}_p)$ in Eq. (29) is the standard construction of the angular momentum vector $\mathbf{J} = 2\mathbf{J}_1$ (with $\tilde{K}_e$ usually regarded as J_z) in terms of the coordinates of an isotropic 2D oscillator. The analogy between the dynamics of a rotator and that of an isotropic 2D oscillator with conserved total action follows from the isomorphism of their algebras, su(2)$\sim$so(3) [25]. It has been widely discussed on many examples (see discussion in Ref. [4]) and applied in the problems of atom-in-fields [7,26–28].

D. Symmetry properties and integrity basis

Let us now consider the action of the symmetry group G_4 on the reduced phase space $S_2 \times S_2$, i.e., on the vectors $\mathbf{K} = (K_e, K_b, K_p)$ and $\mathbf{L} = (L_e, L_b, L_p)$ whose components are used as dynamical variables. Transformation properties of these variables are summarized in Table I. Using these properties and the basic theory of invariants we construct the set of G_4-invariant polynomials, or the *integrity basis* (IB).

The G_4-invariant IB polynomials are used in our study in two major ways. (i) According to the general statements of the theory of invariants, they are necessary and sufficient to represent a polynomial (power series) expansion of any G_4-invariant function, such as the reduced Hamilton function $H_{\text{n.f.}}$, defined on $\Sigma = S_2 \times S_2$. (ii) These polynomials are invaluable for the description of the action of the G_4 group on Σ.

TABLE I. Transformation properties of the dynamic variables of the n-shell reduced problem under the action of the G_4 group (for two orthogional fields).

	E	$T\sigma^{(eb)}$	$\sigma^{(ep)}$	$TC_2^{(e)}$
K_e	+	+	+	+
K_b	+	+	−	−
K_p	+	−	+	−
L_e	+	+	−	−
L_b	+	+	+	+
L_p	+	−	−	+

1. Construction of the integrity basis (IB)

The IB includes main invariants who can enter in the polynomial expansions in any power, and may also include auxiliary invariants whose power can either be 1 or 0. The theory gives the number of the invariants of both types and specifies their construction. In our case (G_4 acting on $S_2 \times S_2$) there are four main and three auxiliary invariants. More precisely,

power in dynamical variables (K_e, K_b, K_p) and (L_e, L_b, L_p)	number of invariants main	auxiliary
1	2	–
2	2	2
4	–	1

Further choice of the invariant polynomials is ambiguous. We choose

$$K_e, \quad L_b, \quad K_b^2, \quad L_e^2, \tag{34a}$$

as basic invariants and

$$L_p^2 - K_p^2, \quad K_b L_e, \quad (L_p^2 - K_p^2) K_b L_e, \tag{34b}$$

as auxiliary invariants.

2. IB for the C_s restricted problem

The C_s restricted problem has a very simple IB. The reduced phase space S_2 [Sec. II C 1] is of dimension 2 and the two main invariants are, naturally, $\tilde{K}_e$ and $\tilde{L}_b$ in Eq. (29). Except for these and $L_p^2 - K_p^2$, all other invariants of the full problem in Eqs. (34) become identically zero when restricted on the C_s-invariant subspace [cf. Eq. (28)]. The remaining auxiliary invariant $\tilde{L}_p^2 - \tilde{K}_p^2$ is not needed because, as seen from Eq. (33), it depends linearly on $\tilde{K}_e^2$ and $\tilde{L}_b^2$. The absence of auxiliary invariants is a simple consequence of the fact that the group G_4 acts on the space of (L_b, K_e, K_p) as an order-two reflection group (cf. Table I) and the IB for groups generated entirely by reflections contains no auxiliary invariants [29].

3. Application of IB polynomials

We can now represent any G_4-invariant polynomial on Σ using the polynomials (34a) as a sum of terms

$$C^{\{i_1,i_2,i_3,i_4\}}(K, L)\, K_e^{i_1} L_b^{i_2} (K_b^2)^{i_3} (L_e^2)^{i_4}, \tag{35a}$$

with functions

$$C^{\{i\}}(K, L) = c^i + c^i_{2a}(L_p^2 - K_p^2) + c^i_{2b}(K_b L_e) + c^i_4 (L_p^2 - K_p^2)(K_b L_e), \tag{35b}$$

and c^i_{2a}, c^i_{2b}, c^i_4, numerical coefficients.

On the other hand, IB polynomials can be used to label orbits of the G_4 group because invariant polynomials (34a) serve as correctly defined coordinates on the space of group orbits of G_4, the orbifold. Invariant polynomial coordinates are the basis of the geometric representation of different spaces of orbits and their invariant subspaces [1].

E. Parameterization of formal series

All analytical results for the reduced problem, such as the reduced Hamilton function (the normal form $H_{\rm n.f.}$), the explicit construction of the reduced phase space, and, later, the position of the stationary points of $H_{\rm n.f.}$, are formal power series; they follow from the explicit normal form transformation $\mathfrak{L}$, itself a formal power series.

To construct these series we choose a formal universal order-of-magnitude parameter τ in such a way that powers of τ correspond to the orders of the transformation $\mathfrak{L}$, and in particular to the orders of the initial and resulting Taylor expansion of the Hamilton function in the phase-space coordinates $x = (q_1 \dots q_4, p_1 \dots p_4)$. Generally, factors g and f in Eq. (18) suit this purpose: if they are both assumed to be of the order τ, i.e., $g \sim \tau$ and $f \sim \tau$, then $H(x) \sim x^2(1 + \tau x^2 + \tau^2 x^4 + \dots)$.

Our concrete choice of τ is based on the dimensionless field parameters G_s and F_s already discussed in Sec. I A 2,

$$F = \frac{1}{3} F_s S \left(\frac{\omega}{2}\right)^4, \quad G = G_s S \left(\frac{\omega}{2}\right)^3, \tag{36}$$

and the field magnitude

$$S = \left(\frac{2}{\omega}\right)^3 \sqrt{G^2 + \left(3\, F \frac{2}{\omega}\right)^2}, \tag{37}$$

such that

$$\tau = n \frac{\omega}{2} S \approx S\ . \tag{38}$$

As a result, the field parameters g and f in Eqs. (18) and (19) become

$$g = G(\omega/2)^{-2} = G_s S(\omega/2) = G_s \tau/n, \tag{39a}$$
$$f = 3F(\omega/2)^{-3} = 3F_s S(\omega/2) = 3F_s \tau/n. \tag{39b}$$

It is well known that perturbation series for nonintegrable systems do not converge, and therefore, there is no point in any rigorous discussion of the convergence. Instead we use truncated series for our analysis. It is important, however, to find a realistic physical estimate for the largest possible value of the smallness parameters S and τ for which our analysis remains meaningful in the whole range of the relative field strengths F_s and G_s. This estimate can be readily obtained by considering the height of the Stark ionization barrier. Clearly, the normal form formulae should apply only below such barrier.

In the initial coordinates Q of Eq. (3) the saddle point of the crossed field potential lies on the electric field axis, with the profile

$$-\frac{1}{Q_e} + F Q_e + \frac{1}{8} G^2 Q_e^2 = -\frac{\omega^2}{8}. \tag{40a}$$

The same direction in the KS space is defined by

$$q_1 = q_2 = 0, \quad q_3 = q_4 = \sqrt{r/2}, \tag{40b}$$

with the profile

$$\frac{r}{2} - \frac{f r^2}{6} + \frac{g^2 r^3}{32} = \frac{4}{\omega}, \tag{40c}$$

and r defined in Eq. (10b). Note, that due to the scaling in Eq. (17) and the sign of the Stark term in Eq. (3),

$$Q_e = -r/\omega. \tag{40d}$$

In the Stark limit both (40a) and (40c) have one single maximum at some nonzero r; the Zeeman term is of higher power, and it results in a minimum at larger r (and, correspondingly, at lower Q_e). With increasing G the two stationary points become closer, collide and disappear, so that there is no Stark ionization at large G. We are primarily interested in the maximum. Its position is easily found for the lhs of Eq. (40c),

$$r_{\max} = 4 \frac{4f - \sqrt{16 f^2 - 27 g^2}}{9 g^2} = 8 \frac{4F_s - \sqrt{D}}{9 S \omega (1 - F_s^2)}\ . \tag{41}$$

with $D = 43 F_s^2 - 27$. We substitute $r_{\max}$ into Eq. (40c) and find the critical value of S,

$$S_{\rm crit} = \frac{(\sqrt{D} - 4F_s)(70 F_s^2 - 4F_s\sqrt{D} - 54)}{3^6 (F_s - 1)^2 (F_s + 1)^2}\ , \tag{42a}$$
$$\approx \frac{3}{16}\left[1 + 25\,\delta + \frac{3193}{4}\,\delta^2 + \frac{124195}{4}\,\delta^3 + \dots\right], \tag{42b}$$

with $\delta = (1 - F_s)/16$, a parameter of the deviation from the Stark limit ($G_s = 0, F_s = 1$). Note, that the above expression does not explicitly depend on energy (on ω)—all energy dependence is absorbed into S due to the definition (37).

We conclude that the upper limit for the physically meaningful values of our smallness parameter is $S < 3/16$. Equation (37) shows that these values of S can be achieved either at high energies ω and low unscaled field strengths (F, G), or at low energies and high field strengths. In the KS formalism, where the potential is regular at the origin, this relation can also be used to measure the scaled excitation energy in units relative to the height of the Stark barrier.

F. Reduced Hamilton function

To construct the normal form of the Hamilton function (18) we treat its terms of degree 4 and 6 in (q,p) as perturbations of order ϵ and ϵ^2, i.e., $f \sim g \sim \epsilon$. Reduction proceeds with regard to orders in ϵ as a standard Lie transformation [30] $R_8(x) \xrightarrow{\mathfrak{L}} \mathcal{R}_8(y)$. The nonlinear near-identity transformation $\mathfrak{L} : x \to y + \ldots$ (as well as the inverse $\mathfrak{L}^{-1} : y \to x + \ldots$) is obtained explicitly as a formal Taylor series $y = x(1 + \epsilon x + \epsilon^2 x^2 + \ldots)$. The procedure is substantially simplified and sped up in the coordinates of Sec. II B 3, and the calculation up to orders ϵ^4 and ϵ^5 becomes quite routine [31].

To represent the resulting normal form $H_{\text{n.f.}}$ we use the n-scaled $\mathbf{K}, \mathbf{L}$ coordinates (30a) of Sec. II C. In these coordinates, the reduced Hamilton function is represented as a formal series,

$$H_{\text{n.f.}} = 4/\omega \tag{43}$$

$$H_{\text{n.f.}} = 2n\Big(1 + \frac{\tau}{2}H_1 + \frac{\tau^2}{4}H_2 + \frac{\tau^3}{2^5}H_3 + \ldots\Big), \tag{44}$$

where, except for the overall factor $2n$ corresponding to the unperturbed hydrogen atom, all explicit n-dependence is absorbed in the formal parameter τ in Eq. (38) and in the scaled normalized field strengths F_s and G_s in Eq. (39). Since $H_{\text{n.f.}}$ is G_4-invariant (Sec. I C), all resonance terms H_k can be expressed in terms of the G_4-invariant polynomials (integrity basis) defined in Sec. II D,

$$H_1 = G_s L_b - F_s K_e \ , \tag{45a}$$

$$\begin{aligned} H_2 = &-\big[3L_b^2 - 2K_e^2 + 3K_b^2 + 2L_e^2 + 2(L_p^2 - K_p^2) - 3\big]G_s^2/4 + \big(7K_eL_b - L_eK_b\big)F_sG_s/3 \\ &-\big(51K_e^2 - 9L_e^2 + 17\big)F_s^2/36 \ , \end{aligned} \tag{45b}$$

$$\begin{aligned} H_3 = &\, L_b\big(6L_e^2 - 6K_e^2 + 9K_b^2 + 5L_b^2 + 6(L_p^2 - K_p^2) - 9\big)G_s^3 - K_e\big(125 - 43L_e^2 + 125K_e^2\big)F_s^3/9 \\ &+\big[-45K_eL_e^2 + 45K_e^3 - 65K_eK_b^2 + 117K_e - 147L_b^2K_e - 45K_e(L_p^2 - K_p^2) + 48L_b(L_eK_b)\big]F_sG_s^2/6 \\ &-\big[3K_b^2L_b + 87L_e^2L_b - 615K_e^2L_b - 3L_b^3 - 232L_b - 3L_b(L_p^2 - K_p^2) + 108K_e(L_eK_b)\big]F_s^2G_s/18 \ . \end{aligned} \tag{45c}$$

We should remark, that ζ must also be used as an invariant polynomial present in the $H_{\text{n.f.}}$: to obtain the above formulae we first express the result of the Lie transformation in terms of $S_2 \times S_2$ IB polynomials in Eqs. (34) *extended* by the extra main invariant ζ in Eq. (12) and two auxiliary invariants ζK_b and ζL_e. Only then we set $\zeta = 0$.

The procedure to obtain the normal form of the C_s restricted Hamilton function (27) is the same as above, but of course, the calculation is much faster for two degrees of freedom. Furthermore, the resulting normal form depends only on $\tilde{n}$, $\tilde{K}_e$, and $\tilde{L}_b$ in Eqs. (29). In particular ζ is not involved since $\zeta \equiv 0$. The lower orders equal those in Eqs. (45) restricted on the C_s sphere by Eqs. (28) and (33). The fourth order contribution is $\tau^4 2^{-7} \tilde{H}_4$ with

$$\begin{aligned} \tilde{H}_4 = &-\frac{17815}{216}F_s^4\tilde{K}_e^4 + \frac{2468}{9}G_s\tilde{L}_bF_s^3\tilde{K}_e^3 - \frac{39685}{108}G_s^2\tilde{L}_b^2F_s^2\tilde{K}_e^2 + \frac{2047\,G_s^2 + 49}{9}G_s\tilde{L}_b^3F_s\tilde{K}_e - \frac{368 + 3853\,G_s^2}{72}G_s^2\tilde{L}_b^4 \\ &+\frac{48218\,G_s^2 - 17815}{108}F_s^2\tilde{K}_e^2 - \frac{17297\,G_s^2 - 7886}{27}G_s\tilde{L}_bF_s\tilde{K}_e + \frac{27152\,G_s^2 - 13787}{108}G_s^2\tilde{L}_b^2 \\ &-\frac{2095}{18}G_s^4 + \frac{4523}{54}G_s^2 - \frac{3563}{216}. \end{aligned} \tag{46}$$

III. GENERAL PROPERTIES OF THE REDUCED PHASE SPACE RELATED TO SYMMETRY

Our present problem, the hydrogen atom in the presence of two external orthogonal fields, is a member of a wider atom-in-fields family [1,2]. In the n-shell approximation all problems in this family have the same reduced phase space $\Sigma = S_2 \times S_2$, but differ in the symmetry properties associated with the particular field configuration [1]. The two factors, the geometry of Σ and the symmetry $\mathfrak{G}$, result in certain important generic features of any Hamilton function $H_{\text{n.f.}}$ on Σ. These general properties are universal, they can be established without any particular (analytic) form of the function $H_{\text{n.f.}}$ [such as in Eqs. (43) and (45)].

A. Invariant subspaces of $S_2 \times S_2$ in the presence of the G_4 symmetry

The main consequence of the presence of additional symmetry is that the phase space Σ is not homogeneous, the points of this space can have different local symmetry, or the stabilizer $\mathfrak{g}$. In the presence of G_4 we can distinguish five different types of points on the reduced phase space $S_2 \times S_2$ with local symmetry $\mathfrak{g} = G_4$, C_s, $\mathcal{T}_s$, $\mathcal{T}_2$, and C_1 (generic points with no symmetry). These points lie on the invariant submanifolds of $S_2 \times S_2$. The latter are described in more detail in Appendix A.

The $S_2 \times S_2$ itself consists of "mostly" generic points and thus can be considered as a C_1 invariant manifold.

This manifold contains four submanifolds. Three submanifolds, invariant with regard to $\mathfrak{g} = C_s$, $\mathcal{T}_s$, and $\mathcal{T}_2$, include all points with their respective local symmetry $\mathfrak{g}$ and all points with higher symmetry G_4. In other words, the G_4-invariant (the fourth) submanifold belongs necessarily to the intersection of the C_s, $\mathcal{T}_s$, and $\mathcal{T}_2$ invariant submanifolds.

Table II summarizes the algebraic description of all these invariant submanifolds. For each submanifold we define the components of $\mathbf{K}$ and $\mathbf{L}$ which must vanish to satisfy the particular local symmetry (cf.Table I), and then simplify general Eqs. (30) which define the whole $S_2 \times S_2$ manifold in the six-dimensional Euclidean space $R_6(\mathbf{K}, \mathbf{L})$ (last column in Table II). These simplified equations demonstrate the topology of the submanifold. Thus, the set of G_4 invariant points forms a one dimensional circle S_1; the C_s as well as the $\mathcal{T}_2$ invariant manifold is a two-dimensional sphere S_2. The $\mathcal{T}_s$ invariant subspace is a two-dimensional torus whose two principal circles can be represented using the e, b-components of $\mathbf{J}_1$ and $\mathbf{J}_1$ [cf. Eq. (31)]. The G_4 invariant circle is, of course, invariant with regard to any subgroup of G_4, and is part of all of the above submanifolds. From the explicit formulae in Table II) we can easily see that this circle is the intersection of the C_s, $\mathcal{T}_s$, and $\mathcal{T}_2$ invariant submanifolds.

TABLE II. Invariant manifolds for the action of the symmetry group G_4 on the reduced phase space Σ.

stabilizer	dim	topology	defining equations	restriction $R_6(\mathbf{K}, \mathbf{L}) \to \Sigma$
G_4	1	S_1	$L_e = K_b = L_p = K_p = 0$	$L_b^2 + K_e^2 = 1$
$C_s = \{E, \sigma^{(ep)}\}$	2	S_2	$L_e = K_b = L_p = 0$	$L_b^2 + K_e^2 + K_p^2 = 1$
$\mathcal{T}_2 = \{E, TC_2\}$	2	S_2	$L_e = K_b = K_p = 0$	$L_b^2 + K_e^2 + L_p^2 = 1$
$\mathcal{T}_s = \{E, T\sigma^{(eb)}\}$	2	$T_2 = S_1 \times S_1$	$L_p = K_p = 0$	$(L_e \pm K_e)^2 + (L_b \pm K_b)^2 = 1$
C_1	4	$\Sigma = S_2 \times S_2$		$\mathbf{L}^2 + \mathbf{K}^2 = 1, \quad (\mathbf{L} \cdot \mathbf{K}) = 0$

B. The special role of time reversal

When, as in our case, symmetry operations involve time reversal, the meaning of various invariant manifolds can be rather different. We must distinguish the invariant manifolds whose stabilizers $\mathfrak{g}$ include purely spatial symmetry operations from those invariant manifolds whose stabilizers include time reversal itself or in combination with spatial operations, such as $T\sigma$ and TC_2 introduced in Sec. I A 2.

For the analysis of the stationary points of the reduced Hamiltonian function $H_{\text{n.f.}}$ (or any other G_4-invariant function) all invariant submanifolds are equally important. Thus to simplify the search for the stationary points we can restrict the $H_{\text{n.f.}}$ on any of the invariant submanifolds. If a point is found, it will automatically be stationary for the $H_{\text{n.f.}}$ defined on the whole Σ. (The gradient of $H_{\text{n.f.}}$ in the direction orthogonal to the invariant submanifold vanishes.) Furthermore, the special symmetry properties of such stationary point are meaningful regardless of whether they are purely spatial or spatial-temporal: as pointed out in Sec. I B 3 and shall be shown later in Sec. IV, each stationary point on Σ corresponds to a periodic orbit in the original phase space, and this correspondence includes the above symmetry properties.

At the same time, when we analyze the behavior of classical trajectories, or more generally, the flux of the $H_{\text{n.f.}}$ on the reduced phase space Σ, we should consider only purely spatial invariance because the corresponding vector field is only invariant with respect to the spatial symmetry. Therefore, we can restrict the flux of the $H_{\text{n.f.}}$ to a submanifold of Σ whose invariance $\mathfrak{g}$ is purely spatial: the vector field is tangent to such submanifold and all classical trajectories remain on it.

It follows that we can study independently the subset of C_s invariant trajectories. We can also study G_4-invariant trajectories as the subset of all C_s invariant trajectories. (The flux is tangent to the C_s invariant sphere $S_2 \subset \Sigma$, and to the G_4-invariant circle $S_1 \subset S_2$, the "equator" of this sphere.) At the same time, the flux is not tangent to the $\mathcal{T}_s$ and $\mathcal{T}_2$ invariant subspaces and trajectories do not remain on these subspaces.

C. The stationary points of $H_{\text{n.f.}}$ on Σ

Global topological properties of the phase space Σ impose certain restrictions on the number and the type of stationary points of the Hamilton function $H_{\text{n.f.}}$ defined on it. General relations between the topological properties of the manifold and the system of stationary points of any smooth function defined on it is the subject of Morse theory [32]. In the case of a finite group, such as G_4, it is natural to suppose that all stationary points of a generic G_4-invariant function $H_{\text{n.f.}}$ are isolated and nondegenerate [33].

For the G_4-invariant Hamilton function $H_{\text{n.f.}}$ defined on the reduced phase space $\Sigma = S_2 \times S_2$ we consider and combine the topological restrictions on the stationary points for all manifolds listed in Table II. The minimum number and the type of stationary points required by the Morse theory for each of these manifolds individually is

topology	number and type of stationary points		
S_1	$1(+)$,	$1(-)$	
S_2	$1(++)$,	$1(--)$	
T_2	$1(++)$,	$1(--)$,	$2(+-)$
$S_2 \times S_2$	$1(++++)$,	$1(----)$,	$2(++--)$

Thus, any smooth Morse-type function $H_{\mathrm{n.f.}}$ must have at least *four* stationary points on the whole $S_2 \times S_2$, two stable (global maximum and minimum) and two unstable (Morse index 2).

In the presence of the G_4 symmetry the minimum number of stationary points remains the same. In this case, all requirements of the Morse theory for each of the four submanifolds of $S_2 \times S_2$ (Table II) can be satisfied if the two stable points lie on the G_4-invariant circle, and the two unstable points lie on the $\mathcal{T}_s$-invariant torus. (The G_4-invariant circle is common to all other invariant submanifolds and the two stable stationary points on it will automatically satisfy the requirements for both C_s and $\mathcal{T}_2$-invariant spheres, and exhaust the minimum number of stable points on the $\mathcal{T}_s$ invariant torus.) Note that the two unstable points are equivalent: they are mapped into each other by operations TC_2 or $\sigma^{(ep)}$ which belong to G_4 but do not belong to $\mathcal{T}_s$. (These points form a two-point orbit of the action of G_4 on Σ, see Appendix A.)

The described location of the stationary points characterizes the *simplest* Morse type function, i.e., the function with minimal possible number of nondegenerate stationary points, defined on the reduced phase space $S_2 \times S_2$ in the presence of the symmetry G_4. Furthermore, since K_e and L_b are the only linear G_4-invariant polynomials, the first order term in the Taylor series of any generic G_4-invariant analytic function on $S_2 \times S_2$ is $\nu K_e + \mu Lb$ (with nonzero μ and ν), and is of the simplest Morse type. This suggests that in the limit of linearization the normal form of the crossed field problem has only four stationary points. We show in Sec. IV A 1 that this is indeed the case. In general, however, the situation might be more complicated at the limit $\mu = 0$ or $\nu = 0$ and might depend on the quadratic terms.

The positions of stationary points within the corresponding invariant submanifolds are not defined by their symmetry because the group orbits formed by these points are not isolated within their strata (see Appendix A 2). When the parameters of the Hamilton function $H_{\mathrm{n.f.}}$, such as the field strengths G and F, are varied, the stationary points can move within their invariant submanifolds, but they cannot leave these submanifolds.

A qualitative change of this system of four stationary points can occur as a result of a bifurcation at some particular value of the parameters. The number of stationary points cannot become less then four, and the four "principal" stationary points described above cannot disappear. They can, however, change their stability if the Morse theory requirements remain satisfied due to the appearance or disappearance of additional stationary points. Note, that since the two $\mathcal{T}_s$-invariant points are equivalent (they form one group orbit), their bifurcations should be identical, i.e., should occur at the same values of parameters, produce the same local qualitative change, etc. We should further note that due to the special location of the principal stationary points (especially of the two G_4-invariant points), many additional restrictions on possible bifurcations can be deduced from the Morse theory requirements. The bifurcation study of the nonlinear normal modes of the actual crossed field problem requires the stability analysis in Sec. IV E and involves high orders of $H_{\mathrm{n.f.}}$ [34].

IV. NONLINEAR NORMAL MODES DERIVED FROM THE REDUCED PROBLEM

As any other generic G_4-invariant function on the reduced phase space $S_2 \times S_2$, the normal form $H_{\mathrm{n.f.}}$ has four principal stationary points described in Sec. III C. These four relative equilibria correspond to four principal periodic orbits of the initial problem (cf.Sec. I B), the hydrogen atom perturbed by external fields.

The correspondence is comprehensive: the symmetry properties of the orbit and its stability can be deduced from the characteristics of the corresponding stationary point. Furthermore, the action along the orbit and the period can be derived from the normal form in Eqs. (44) and (45) as formal power series in τ (or S) with parameters G_s and F_s. In principle, as we show further below, even the initial (physical three-dimensional) phase-space image of the orbit itself can be reconstructed from the position of the stationary point (on Σ) and the explicit formulae for the transformation (6).

The importance of the four principal stationary points is, as we stress in Sec. III C, that they exist at all possible values of parameters. In particular, only they exist at any infinitesimally small (but nonzero) field parameters. Since the corresponding four families of periodic orbits possess, of course, the same property, we call them nonlinear normal modes.

A. Evolution between the Zeeman and Stark limits

To find what happens in general to the four nonlinear normal modes when the field configuration is changed from the Zeeman to the Stark limit we analyze the behavior of the corresponding four stationary points in the lowest order approximation.

1. Linear approximation

Consider the linear-in-field part of the reduced Hamilton function (43),

$$H_{\mathrm{n.f.}} = 2n\Big[1 + \frac{\tau}{2}(G_s L_b - F_s K_e) + \ldots\Big] = \frac{4}{\omega}. \qquad (47)$$

The calculation of the four stationary points of (47) on $S_2 \times S_2$ is straightforward [use Eqs. (1) and (30a)]. Below we use IB polynomials (34a) and (34b) to characterize the points.

$\mathfrak{g}$	K_e	Kb^2	Le^2	L_b	$K_p^2 - L_p^2$	$H_{\rm n.f.}$
G_4	$-F_s$	0	0	$+G_s$	0	$2(n+\tau)$
G_4	$+F_s$	0	0	$-G_s$	0	$2(n-\tau)$
$\mathcal{T}_s$	0	$(\pm G_s)^2$	$(\mp F_s)^2$	0	0	$2n$

Since the two $\mathcal{T}_s$-invariant points are equivalent (they correspond to the same orbit of the G_4 group action) the values of invariant polynomials are the same. In fact all G_4-invariant characteristics of these two points, such as the value of $H_{\rm n.f.}$, will be the *same* (to any order in τ). On the contrary, the two G_4-invariant points are not equivalent and their characteristics differ.

As expected in Sec. III C, the stationary points of $H_{\rm n.f.}$ change their position without leaving their $\mathfrak{g}$-invariant ($\mathfrak{g} = G_4$ or $\mathcal{T}_s$) subspaces. All the way from the Zeeman to Stark limit the G_4-symmetric stationary points with $L_b \approx G_s$ and $L_b \approx -G_s$ remain the global maximum and minimum of the $H_{\rm n.f.}$ (with $n =$ const, i.e., for one n-shell). At the same time, the two $\mathcal{T}_s$-symmetric stationary points remain unstable. Note that such monotone evolution of the stationary points between the two limits is very different from the case of the two parallel fields [1,3].

2. Properties of nonlinear normal modes

The symmetry properties and stability of the four nonlinear normal modes follow directly from those of the four stationary points. We first consider the situation when both fields are nonzero ($F \neq 0, G \neq 0$) and the symmetry of the problem is precisely G_4.

There is no time reversal symmetry in the problem ($T \notin G_4$) and therefore if the image of a periodic trajectory in the initial physical configuration space R_3 is a loop, it has only one distinct direction.

Furthermore, since each stationary point has a single nonzero component of the orbital momentum $\mathbf{L}$ all corresponding nonlinear normal modes are indeed loops in R_3 (as opposed to lines which run in both directions). From the linear solution (Sec. IV A 1) we conclude that the G_4-type trajectories are loops around axis b ($L_b \neq 0$), while the $\mathcal{T}_s$-type orbits loop mainly around axis e ($L_e \neq 0$).

The G_4-invariant trajectories must lie in the (ep) plane ($Q_b = P_b = 0$) in order to be invariant with regard to $\sigma^{(ep)}$ and hence they necessarily have $L_e = L_p = 0$ (cf. Table II). On the contrary, the $\mathcal{T}_s$-symmetric trajectories have no invariant configuration subspace in R_3 because their stability group is not purely spatial (cf. Sec. III B). These two $\mathcal{T}_s$-trajectories are equivalent: the symmetry operations $\sigma^{(ep)}$ or TC_2 map them into each other.

3. Symmetry of the Zeeman and Stark limits

The symmetry of the two limits is much higher than just G_4 [1,2], it includes the C_∞ element, $C_\infty^{(e)}$ for the Stark and $C_\infty^{(b)}$ for the Zeeman limit. The typical orbit of the C_∞ group action is a circle S_1 (or several S_1's for C_∞ combined with additional finite symmetries) and in addition to simple stationary points the typical Hamilton function defined on $S_2 \times S_2$ in the presence of such symmetry can possess stationary (critical) manifolds S_1 [33]. Four principal stationary points remain simple nondegenerate stationary points in both the Zeeman and Stark limit.

In the Zeeman limit, the two G_4-symmetric stationary points become two critical one-point group orbits with $C_{\infty h} \wedge \mathcal{T}_s$ symmetry. These orbits correspond to the maximum and minimum L_b. (The linear Zeeman effect and the C_∞ symmetry are not reduced!.) In the initial physical coordinate space R_3, the corresponding periodic trajectories run in two different directions along two circles lying in the plane orthogonal to the field axis and having different radii (see Fig. 2).

In the Stark limit, the same two G_4-symmetric stationary points become two critical one-point orbits with $C_{\infty v} \wedge \mathcal{T}$ symmetry. They now are invariant with respect to time reversal, and their coordinate space image (in R_3) is a line. There are two lines with $C_{\infty v}$ symmetry: “up” and “down” the electric field F on the e-axis (Fig. 2). The “down-hill” trajectory is longer than the “up-hill” one, has higher (maximum) energy at the same n and ionizes at sufficiently high field.

The two $\mathcal{T}_s$-symmetric stationary points form one two-point orbit of the G_4 symmetry group action. They remain equivalent in both the Zeeman and the Stark limit. In the Zeeman limit these two points form one two-point critical orbit of the $C_{\infty h} \wedge \mathcal{T}_s$ group action with stabilizer $\mathfrak{g} = C_\infty \wedge \mathcal{T}_s$. In this limit they have $\mathbf{L} = 0$ and hence their images in R_3 are two lines lying on the b-axis up and down the magnetic field (see Fig. 3). The two lines are equivalent, the $\sigma_h = \sigma^{(ep)}$ operation maps them into each other.

In the Stark limit the same pair of equivalent $\mathcal{T}_s$-symmetric points becomes one two-point orbit with the $\mathfrak{g} = C_\infty \wedge \mathcal{T}_s$ symmetry. In R_3, these are circles around the e-axis lying in the plane orthogonal to the e-axis ($Q_e =$ const $\neq 0$, see Fig. 3).

The appearance and breaking of the C_∞ group orbits, in particular the stationary S_1 manifolds, and of the foliation of $S_2 \times S_2$ corresponding to the additional integral of motion (L_b or L_e) in the Zeeman and Stark limit require separate detailed analysis.

B. Position of stationary points

As we already know from the linear solution (Sec. IV A 1), no stationary point in the problem with two crossed fields has fixed position on Σ. Therefore we first find the position of the four stationary points as function on F and G. As everything else, this function is obtained analytically as a formal power series in an appropriate smallness parameter. The order of this series is limited by the order to which the normal form itself is developed, such as order 3 in the case of Eqs. (43), (44), and (45).

1. The choice of formal parameter

Periodic orbits of nonintegrable systems are studied at given fixed energy $E=$ const. In the presence of an approximate integral, such as n, the energy remains a preferred parameter when an exact (numerical) orbit is sought or in the transition-to-chaos region where the n-shell approximation is expected to break. Consequently, in this section we take the energy E as an independent parameter when we compute the characteristics of periodic trajectories, such as action and period,

Furthermore, we take scaled strengths F_s and G_s and the field magnitude S defined in Eqs. (37) and (36) as our field parameters. These parameters are scaled by $\omega(E)$, and thus are fixed at given F, G, and E. The formal series parameter τ of the normal form (44) is expressed in terms of S, ω, and n [Eq. (38)].

On the other hand, the whole concept of the reduced phase space Σ and of relative equilibria, the stationary points points on Σ is valid only if n can be regarded as an integral of motion. Consequently, it makes more sense to rely directly on n (or τ) as an independent parameter when we compute the characteristics of these equilibria. Indeed, the coordinates on $\Sigma=S_2\times S_2$, and hence the coordinates of the stationary points, are the n-scaled components of vectors $\mathbf{K}$ and $\mathbf{L}$ defined in Eqs. (30) and (1). The other advantage to have n as an independent parameter in the reduced problem is the simple possibility to pass to the corresponding quantum system using the semiclassical (EBK) quantization of n.

As a result, depending on the application, we use either n (or τ) or E (or S) as an appropriate independent parameter in addition to the field strengths G and F. This, of course, requires the ability to change between the two parameter schemes, and in particular—to find the value of n at given $\omega(E)$ and $\{S,F_s,G_s\}$.

2. The value of n as function of energy and field strengths

The principal integral of motion n as function of energy E [or $\omega(E)$], $S_2\times S_2$ coordinates $(\mathbf{K},\mathbf{L})$ and field parameters (S,F_s,G_s) is defined implicitly by the constant level set equation

$$H_{\rm n.f.}(\mathbf{K},\mathbf{L};\,n,\tau,F_s,G_s)=\frac{4}{\omega(E)}=\text{const.} \tag{48}$$

Remember, that we use normalized vectors $\mathbf{K}$ and $\mathbf{L}$ [Eq. (30a)], and all dependence of the $H_{\rm n.f.}$ in Eq. (48) [in Eqs. (43) and (45)] on n is concentrated in the parameter τ. We solve (reverse) Eq. (48) as a formal power series in S: we multiply Eq. (44) by $\frac{1}{4}S\omega$ so that

$$S=\tau+\frac{\tau^2}{2}H_1+\frac{\tau^3}{4}H_2+\frac{\tau^4}{32}H_3+\dots \tag{49a}$$

and consequently

$$\begin{aligned}\tau=S-\frac{S^2}{2}H_1+\frac{S^3}{4}(2H_1^2-H_2)\\ -\frac{S^4}{32}\Big[20H_1(H_1^2-H_2)+H_3\Big]+\dots\ ,\end{aligned} \tag{49b}$$

with functions H_k given by Eqs. (45) above. From Eq. (38) we see immediately that

$$n=\frac{2}{\omega}\left[1-\frac{S}{2}H_1+\frac{S^2}{4}(2H_1^2-H_2)+\dots\right]. \tag{49c}$$

At this point Eq. (49c) appears as a formal result of our parameterization scheme. We analyze the dynamical meaning of this expression in Sec. IV C below.

3. Formal series for the position of stationary points

To compute the position of the four principal stationary points in Sec. III C we look for the extrema of either the normal form $H_{\rm n.f.}(\mathbf{K},\mathbf{L};\tau,n,G_s,F_s)$ in Eqs. (44) and (45), i.e., the energy E, or the value of $n(\mathbf{L},\mathbf{K};E,G,F)$ in Eq. (49c). In each case the coordinates $(L_e,L_b,L_p,K_e,K_b,K_p)$ of stationary points obey the condition $\nabla F=0$, with $F=H_{\rm n.f.}$ or n, and with additional restrictions (30) imposed on the six components of the gradient by the $S_2\times S_2$ topology. In other words we should solve the system of equations

$$\nabla_{\mathbf{K},\mathbf{L}}F=0,\quad \mathbf{K}^2+\mathbf{L}^2=1,\quad \mathbf{K}\cdot\mathbf{L}=0. \tag{50}$$

The formal series solutions to Eqs. (50) are obtained by the Newton's method with four linear solutions in Sec. IV A 1 used as germs to start nonlinear series in τ if $F=H_{\rm n.f.}$, or S if $F=n$. Since $H_{\rm n.f.}$ in Eqs. (45) is obtained to the third order in τ, three will be the order of the rest of our formulae, such as (49c) and those below.

We determine the positions $\{\mathbf{K},\mathbf{L}\}_{\rm st.p.}$ of the four stationary points using $H_{\rm n.f.}$ as F in Eqs. (50). This yields formal series with τ, i.e., n, as a parameter. Then, at each particular stationary point $\{\mathbf{K},\mathbf{L}\}_{\rm st.p.}$, we use the method in Sec. IV B 2 to find the value of n at given energy E as a solution to Eq. (48). Thus we obtain $n(S(E))_{\rm st.p.}$ as a formal power series in S. Results are shown in Table III.

TABLE III. Position of the stationary points on $S_2 \times S_2$ and the action n of the corresponding trajectories.

$\mathfrak{g}$[a]	[b]	low order	high order
G_4	K_e	$\mp F_s - \tau F_s G_s^2(4G_s^2-3)/12$	$\mp \tau^2 F_s G_s^2(-103G_s^2 - 60G_s^4 + 40G_s^6 + 21)/144$ $- \tau^3 F_s G_s^2(2^9 G_s^{10} - 1152G_s^8 - 1500G_s^6 + 5261G_s^4 - 6823G_s^2 + 2010)2^{-6}3^{-3}$
	L_b	$\pm G_s - \tau G_s F_s^2(4G_s^2-3)/12$	$\mp \tau^2 G_s F_s^2(80G_s^6 - 104G_s^4 - 230G_s^2 + 51)/288$ $- \tau^3 G_s F_s^2(2^{10} G_s^{10} - 2^{11} G_s^8 - 3512G_s^6 + 9806G_s^4 - 12725G_s^2 + 3867)2^{-7}3^{-3}$
	$\frac{1}{2}n\omega$	$1 \mp S/2$	$+ S^2(G_s^4/4 - 5G_s^2/3 + 35/12)/3$ $\pm S^3(G_s^8/3 - G_s^6/2 - 35G_s^4/4 + 35G_s^2 - 385/12)/12$ $+ S^4(4G_s^{12}/9 - G_s^{10} - 70G_s^6/9 - 41G_s^8/8 + 1771G_s^4/12 - 1001G_s^2/3 + 5005/24)/24$
T_s	K_e	$- \tau F_s G_s^2(4G_s^2+1)/12$	$- \tau^3 F_s G_s^2(126G_s^2 + 1025G_s^4 - 1500G_s^6 - 64G_s^8 + 2^9 G_s^{10} - 108)2^{-6}3^{-3}$
	L_b	$- \tau G_s F_s^2(4G_s^2+1)/12$	$- \tau^3 G_s F_s^2(2^{10} G_s^{10} + 2^7 G_s^8 - 2680G_s^6 + 1526G_s^4 + 157G_s^2 - 203)2^{-7}3^{-3}$
	K_b	$\pm Gs$	$\mp \tau^2 G_s F_s^2(80G_s^6 + 72G_s^4 - 146G_s^2 + 13)/288$
	L_e	$\mp Fs$	$\mp \tau^2 F_s G_s^2(6 - 77G_s^2 + 28G_s^4 + 40G_s^6)/144$
	$\frac{1}{2}n\omega$	1	$- S^2 F_s^2(3G_s^2-2)/36$

[a]Local symmetry (stabilizer) of the stationary point.
[b]Only nonzero components of **K** and **L** are given.

C. Action and period

Each point of the reduced phase space $\Sigma = S_2 \times S_2$ corresponds to a set of points on the initial phase space R (or $\mathcal{R}$). By construction, all these points correspond to the same value of the principal integral n in Eqs. (20) and (1). In other words, each point of Σ defines an orbit of n in R. (As outlined in Sec. I B, n defines a dynamical symmetry operation with linear action in R_8.) The conjugated angle ϕ_n is the natural coordinate along these orbits.

On the reduced phase space Σ, the dynamics of the system is described by the Hamilton function $H_{\text{n.f.}}$ in Eqs. (43), (45) and (48). To find the trajectory in the initial phase space R we combine the trajectory on the Σ with the n-orbit motion (cf. the general outline in Sec. I B 3). In the particular case of a stationary point of $H_{\text{n.f.}}$ we obtain a periodic trajectory in R with ϕ_n the coordinate along it. (In other words, the n-orbit in this case corresponds to an actual periodic orbit of the system.)

The coordinates $\{\mathbf{K}, \mathbf{L}\}_{\text{st.p.}}$ of the stationary point and the value of n at this point can be expressed as functions of $\omega(E)$ and G_s, F_s, S. At the same time the Hamilton function $H_{\text{n.f.}}$ at this point defines a one-dimensional dynamical system with (n, ϕ_n) the action-angle variables and ϕ_n the ignorable angle. Then it follows immediately (see, for instance, Chap. 10 §50B of Ref. [35]) that

$$n_{\text{stationary point}} = \frac{1}{2\pi} \oint_{\text{periodic orbit}} \mathbf{p}\, d\mathbf{q} \, , \tag{51}$$

with the action integral defined in terms of the KS phase space $R_8 = \{q_1, q_2, q_3, q_4, p_1, p_2, p_3, p_4\}$ [cf. Eqs. (10) and (11)]. Since the normal form transformation $\mathfrak{L}$ [Eq. (6)] is canonical this integral is the same for R_8 and $\mathcal{R}_8$, but the action integral on the initial physical space $R_6 = \{Q_e, Q_b, Q_p, P_e, P_b, P_p\}$ is different.

We can now understand the dynamical meaning of Eq. (49c), the solution $n(E)$ of (48). This equation gives the value of the action integral along an n-orbit in the R_8 (or the $\mathcal{R}_8$) space at given energy E, field strengths F, G, and given (fixed) vectors $(\mathbf{L}, \mathbf{K})$. The periodic orbits correspond to the extrema of $n(E)$. In fact, the extremal values of the action integral (51) are already derived as functions of energy in Sec. IV B 3 and Table III.

To calculate Δ, the KS space period of periodic orbits, we begin with its definition and use Eqs. (38) and (43) to obtain

$$\frac{\Delta}{2\pi} = \left[\frac{dH_{\text{n.f.}}}{dn}\right]^{-1} = \left[\frac{dH_{\text{n.f.}}}{d\tau} S \frac{\omega}{2}\right]^{-1} = \frac{1}{2}\left[\frac{d}{d\tau}\left(H_{\text{n.f.}} S \frac{\omega}{4}\right)\right]^{-1} = \frac{1}{2}\left[\frac{dS}{d\tau}\right]^{-1} = \frac{1}{2}\frac{d\tau}{dS} = \frac{1}{2}\frac{d}{dS}\left(n\frac{\omega}{2}S\right) , \tag{52}$$

with functions $H_{\text{n.f.}}$, $S(\tau)$, and $\tau(S)$ evaluated at the stationary point. In other words, we find the period Δ/π by taking the derivative of $\frac{1}{2}n\omega$ times S. Therefore, the period is approximated with lesser accuracy than the action for the same order of the normal form.

In Fig. 1 we compare our normal form predictions shown by lines with the numerically refined "exact" values shown by circles. We consider all values of the field strength S that cause no ionization in the Stark limit ($G_s = 0$) and tune the system towards the Zeeman limit ($F_s = 0$). The last set of data is taken at $S = 0.18$ with energies about 95% of the ionization threshold ($S = 3/16$) of the regularized Hamilton function (18).

The action n and the period Δ/π of the T_s orbits is well reproduced in the whole range of S already in the third order. The approximation for the G_4 orbits is less accurate. At large values of S the series for the ionizing orbit is about to diverge and high order corrections are needed to achieve reasonable reproduction of the numerical data. We show the result of successive approximations obtained for this orbit in orders $4, 5, 6, 7, 8$ from the C_s restricted normal form. [The fourth order is given in Table III, higher order formulae are too large to be reproduced there.] The series for the non-ionizing G_4 orbit is alternating (cf. Table III). When S is large, this series wildly oscillates in low orders and settles only at orders higher than 4.

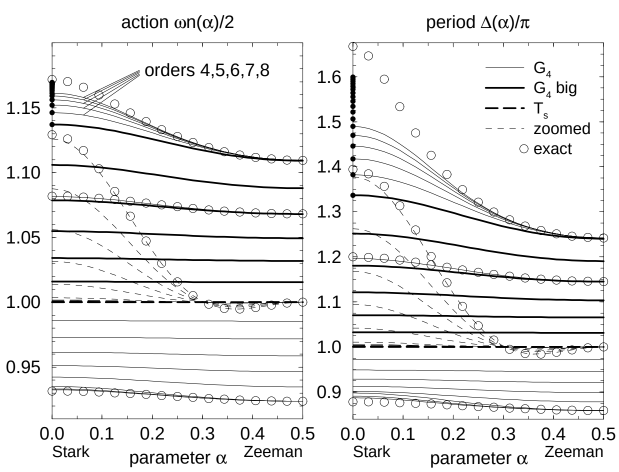

FIG. 1. Action and period of the nonlinear normal modes in the whole range between the Stark ($\alpha = 0$) and Zeeman ($\alpha = \frac{1}{2}$) limit with $F_s = \cos(\alpha\pi)$, $\omega = 2$ ($n \sim 1$), and $S = 0.03, 0.06, 0.09, 0.12, 0.15, 0.18$. Lines, bold for downhill (big) G_4 orbit, thin for uphill (small) G_4 orbit and dashed for $\mathcal{T}_s$ orbit, show order 3 approximation of Table III. Empty circles show exact numerical results. Data for $\mathcal{T}_s$ orbits are blown up by factor of 70. Approximations of orders $4 \dots 8$ for the G_4 orbits with $S = 0.18$ are shown in the whole range of α by thin lines. Black dots on the $\alpha = 0$ axis show successive 1D normal form approximations of orders $4 \dots 20$ for this orbit in the pure Stark limit with $S = 0.18$ (96% of the ionization threshold).

To understand if the perturbation series could reach better accuracy at $S = 0.18$ we calculated the normal form for the ionizing G_4 orbit in the pure Stark limit where this orbit is a straight line and the problem reduces to one degree of freedom. Figure 1 demonstrates that even at order of 20 the discrepancy is large! The reason for such sluggish convergence is most likely due to the "nongeneric" potential barrier with no q^3 terms [Eq. 40c].

D. Periodic orbits in the initial space R

In this section we make the correspondence between the stationary points of the normal form $H_{\text{n.f.}}$ and the nonlinear normal modes explicit and complete by finding the trajectories of these modes in the initial phase space R_6. The procedure has three main steps: we first find the correspondence between the reduced space $S_2 \times S_2$ and the transformed space $\mathcal{R}_8$, i.e., the embedding of $S_2 \times S_2$ into $\mathcal{R}_8$, then we return to the initial phase space R_8 using explicit formulae of the Lie transformation $\mathfrak{L}^{-1}$ obtained in Sec. II F [cf. Eq.(6)]; and finally we use KS expressions in Sec. II B to map from R_8 to R_6, the phase space of the initial 3D Hamilton function (3).

Our first step gives an opportunity to review once again the geometry of the problem. We lifted the initial physical phase space R_6 [or C_3 defined in terms of complex coordinates $q \pm ip = \sqrt{2I}\exp(\pm\phi)$] to the KS space R_8, transformed the latter into $\mathcal{R}_8$ and then reduced to Σ_4, a four dimensional space with topology $S_2 \times S_2$. We also defined the standard dynamical coordinates $\mathcal{R}_8 \to \mathcal{R}'_8$ in Sec. II B 3 in which the two group actions defined by n and ζ are diagonal. To find the embedding of Σ into $\mathcal{R}_8$ we need local charts of Σ in terms of coordinates on $\mathcal{R}'_8$, i.e., in terms of $(q'_1, q'_2, q'_3, q'_4, p'_1, p'_2, p'_3, p'_4)$. Each chart is a Euclidean space $\mathcal{R}'_4$. /* cpp: beware of single quotes ... */ The atlas sufficient to cover the whole of $S_2 \times S_2$ consists of four such charts. Below we give the explicit construction of this atlas.

The normal form reduction $R_8 \to \mathcal{R}_8 \sim \mathcal{C}_4$ of the KS Hamilton function (18) with regard to n leads in fact to a standard definition of a complex projective space $\mathcal{C}_4 \to CP_3$. The image of each point on CP_3 is an orbit in $\mathcal{C}_4$, and the phase ϕ_n, the ignorable angle variable, is the coordinate along this orbit [36]. In addition to n the problem (18) has one exact integral ζ which defines the action of an SO(2) symmetry group of Eq. (18) on R_8. Generic points on the reduced space $S_2 \times S_2$ correspond to a torus with phase coordinates ϕ_n and ϕ_ζ. In other words, the group action defined by both n and ζ is reduced.

Consequently, to find the image of a point on $S_2 \times S_2$ with coordinates $(\mathbf{K}, \mathbf{L})$ in the KS space R_8 we should define the values of two phase variables ϕ_n and ϕ_ζ. The phase ϕ_n is the coordinate along the periodic trajectory we want to construct (cf. Sec. I B 3), it changes on the interval $[0, 2\pi]$. The phase ϕ_ζ has no importance to us: all points on the same ζ-orbit in $\mathcal{R}_8$, a circle S_1, will eventually be mapped into one point of the physical space R_6. So we can fix ϕ_ζ to some value, for instance 0.

In the standard diagonal representation of Sec. II B 3 phases ϕ_n and ϕ_ζ are simply expressed in terms of angle variables ϕ_i of the four oscillators $p_i'^2 + q_i'^2$, $i = 1, \dots, 4$,

$$\phi_n = \tfrac{1}{2}(\phi_1 + \phi_2 + \phi_3 + \phi_4), \tag{53a}$$

$$\phi_\zeta = -\phi_1 - \phi_2 + \phi_3 + \phi_4 \ . \tag{53b}$$

To lift Σ to $\mathcal{R}'_8$ we can fix any two phases in Eqs. (53). Thus we can fix ϕ_a and ϕ_b and obtain the chart $M^{(ab)}$: $p_b = p_a = 0$. Such chart covers all points except for those where n_a and/or n_b vanish and phases ϕ_a and/or ϕ_b become undefined. In particular, it is the only chart that covers the subspace where two other actions, n_c and n_d, vanish and $n_a + n_b = n$. Equation (25b) shows that four such pairs (cd) exist if $\zeta = 0$ and $n \neq 0$ ($n = 1$ in the scaled coordinates). Therefore, four charts with

$$(ab) = (13), (23), (14), (24), \tag{54}$$

are required. It can also be shown that these four charts are sufficient to cover the whole $S_2 \times S_2$.

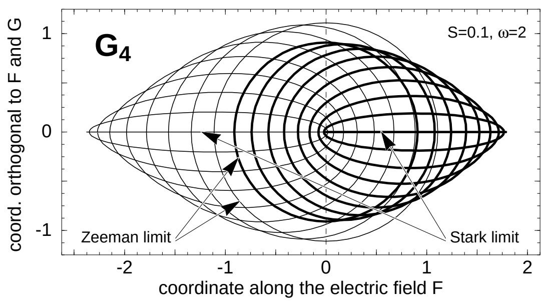

FIG. 2. Projections of the two G_4 orbits at different F_s and G_s, for $S = 0.1$ and $\omega = 2$ ($n \sim 1$).

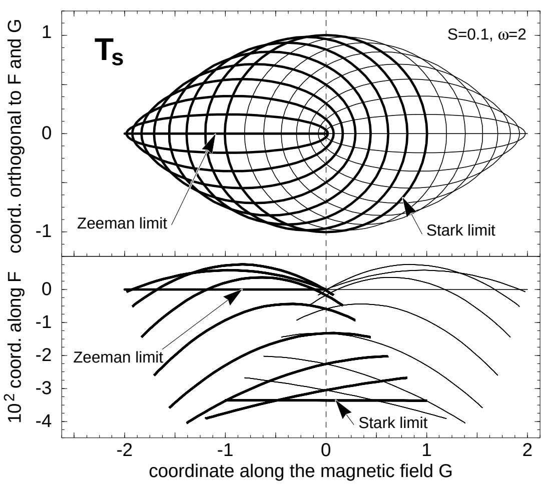

FIG. 3. Projections of the two equivalent T_s orbits at different F_s and G_s, for $S = 0.1$ and $\omega = 2$ ($n \sim 1$).

To find the image of the stationary points in Table III we first obtain the values of n_1, n_2, n_3, n_4 using Eqs. (25) with $\zeta = 0$ and $n = 1$. Thus in the linear approximation of Sec. IV A 1 we obtain

$\mathfrak{g}$	$2n_1$	$2n_2$	$2n_3$	$2n_4$
G_4	$1 \mp G_s$	$1 \pm G_s$	$1 \mp G_s$	$1 \pm G_s$
$\mathcal{T}_s$	$1 \mp G_s$	$1 \pm G_s$	$1 \pm G_s$	$1 \mp G_s$

.

We choose a pair in Eq. (54) with largest values of (n_a, n_b) and define the corresponding chart of $S_2 \times S_2$. In principle, we can follow the whole periodic orbit in this chart by varying ϕ_n. On the other hand, to demonstrate the validity and accuracy of the normal form prediction, we can simply fix two phases $\phi_a = \phi_b = 0$, generate one point on this orbit as the initial condition in R_8, and then propagate the orbit numerically using the exact Hamilton function (18).

Results of such calculation are shown in Figs. 2, 3, and 4. The former two figures show the projections of the orbits on the planes in the initial 3D configuration space. The orbits are tuned between the Zeeman and Stark limits at moderate perturbation $S = 0.1$ ($\sim 50\%$ of the Stark ionization threshold). Their images exhibit all symmetry properties expected in Sec. IV A 2. In particular, the G_4-orbits lie in the (ep)-plane while the $\mathcal{T}_s$-orbits are lightly curved. The global view of all four orbits in the 3D configuration space is given in Fig. 4.

E. Stability

To conclude our study of the nonlinear normal modes of the crossed fields problem we analyze their stability. The geometric characteristics of stability is given by the eigenvalues of the Hessian matrix; for qualitative purposes we only need to know the signs of these eigenvalues, i.e., the signature of the Hessian matrix. The dynamical characteristics of stability is given by the linear Hamilton equations describing the motion near the orbit, in particular, by the frequency of oscillations near a stable orbit.

Using the Morse theory we have already shown in Sec. III C that G_4 symmetric stationary points on Σ are stable, one is a global minimum with the signature $(++++)$, the other is a global maximum $(----)$. Of course, the two corresponding periodic orbits are also stable. Furthermore, by the simple argument of the length of the orbit it is the larger or “downhill” G_4 orbit which has the maximum action. When this orbit escapes, the action becomes infinite. The two equivalent $\mathcal{T}_s$ symmetric points and the corresponding periodic orbits are unstable.

The position of the stationary point on $S_2 \times S_2$ in the J-representation (31) is defined by four spherical angle coordinates (φ_i, θ_i), $i = 1, 2$, such that, for instance,

$$\cos\theta_i = 2J_{ip}, \quad \sin\theta_i = 2\sqrt{J_{ie}^2 + J_{ib}^2}, \tag{55}$$

and similarly for $\sin\varphi_i$ and $\cos\varphi_i$ [cf.Eq. (32)]. The Hessian matrix is the 4×4 matrix of second derivatives of $H_{\text{n.f.}}$ in Eq. (43) with regard to the coordinates on the hyperplane tangent to $S_2 \times S_2$ at this point. We construct the tangent coordinates (J_{ix}, J_{iy}) by appropriately rotating the standard frame,

$$(J_{ie}, J_{ib}, J_{ip}) \to (J_{ix}, J_{iy}, J_{iz}), \quad i = 1, 2. \tag{56}$$

The normal component J_{iz} is expressed in terms of $(J_{1x}, J_{1y}, J_{2x}, J_{2y})$ using Eq. (32) and the derivatives are calculated.

TABLE IV. Stability characteristics of the nonlinear normal modes.

$\mathfrak{g}$[a]	Hessian[b]	frequencies[c] ω', ω''
G_4	$[+\tau, +\tau, +\tau, +\tau]$	$+\tau + \tau^2(G_s^4 - 7G_s^2/3 + 17/6)/2$
G_4	$[-\tau, -\tau, -\tau, -\tau]$	$-\tau + \tau^2(G_s^4 - 7G_s^2/3 + 17/6)/2$
T_s	$[-\tau, +\tau, -\tau, +\tau]$	$\pm\tau + \tau^2(G_s^4 + G_s^2 - 1/2)/2$
T_s	$[+\tau, -\tau, +\tau, -\tau]$	$\mp\tau + \tau^2(G_s^4 + G_s^2 - 1/2)/2$

[a] local symmetry group of the stationary point
[b] the eigenvalues of the Hessian matrix in the coordinates $(J_{1x}, J_{2x}, J_{1y}, J_{2y})$ in the linear approximation
[c] For each G_4 mode ω' equals ω''.

Two Euler rotations, first by angle φ_i and then by angle θ_i are required. It turns out that the third Euler rotation, a rotation of the tangent plane around axis J_{iz}, is not required because the Hessian matrix comes out already factorized. In the lowest (linear-in-τ) order this matrix is diagonal (see Table IV), in higher orders it requires additional transformation of each of the (J_{1x}, J_{2x}) and (J_{1y}, J_{2y}) blocks. For the G_4 points this latter factorization simply results in the coordinates (K_x, L_x) and (K_y, L_y).

Furthermore, the canonical structure $dJ_{1x} \wedge dJ_{1y} + dJ_{2x} \wedge dJ_{2y}$ is preserved by the above factorization and defines the normal modes of the oscillations near each stationary point (periodic orbit) and their frequencies ω', ω''. The values of ω', ω'' calculated up to order $O(\tau^3)$ are shown in Table IV. For moderate values of $\tau \sim S < 3/16$ the stability of the orbits does not change qualitatively. We should, however, bear in mind, that, as given by Eq. (38), τ depends on n. The required value of n is the action for the corresponding orbit listed in Table III.

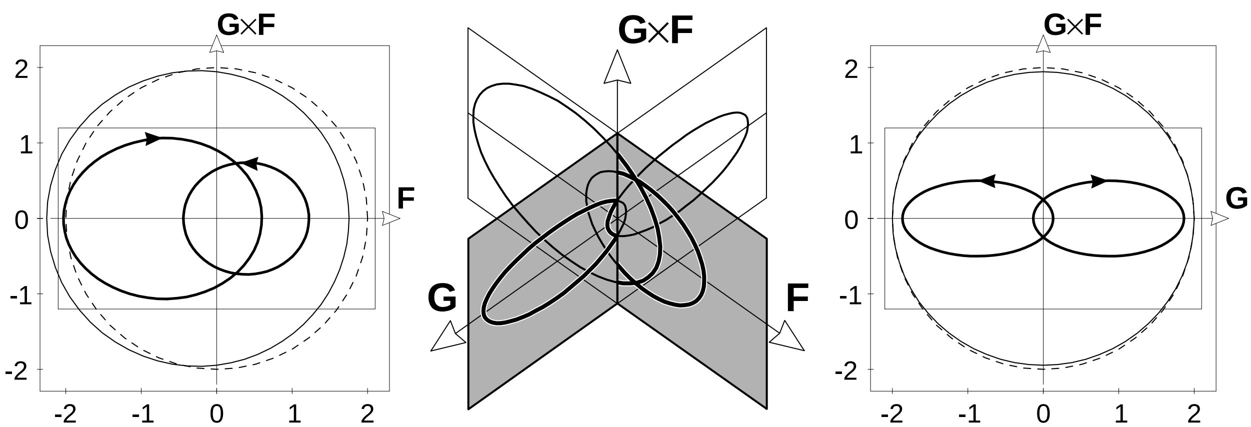

FIG. 4. Nonlinear normal modes of the crossed fields problem at $S = 0.2$, $F_s = \cos(\pi/3)$, and $\omega = 2$ ($n \sim 1$). Rectangles on the left and right plots correspond to those in the center. A circle shown by broken line gives the value of the unperturbed (Coulomb) potential, while the solid line circle gives the actual potential. The arrows on the orbits show their "direction" required to analyse their time-reversal symmetry.

V. DISCUSSION

This paper presents a complete analytic study of the nonlinear normal modes (NNM's) of one particular problem, the hydrogen atom in crossed electric and magnetic fields. We reduce our problem with regard to the principal Coulomb integral n and derive all information on the main periodic orbits by studying the stationary points (the relative equilibria) of the corresponding n-shell reduced Hamilton function.

The main general value of this work is in the unified approach to the analysis of NNM's: we explicitly combine the periodic orbit study with the reduction methods and concepts of modern nonlinear dynamical theory. Our approach leads to the idea of tuning the crossed fields problem in the whole range between the two limit configurations while remaining at the same level of the combined perturbation by the two fields, and to the appropriate scaling and parameterization. The realization of this idea is an important contribution to the crossed fields problem.

NNM's are the most basic elements of the dynamical structure on the phase space associated with the particular dynamical nonlinear system. Their existence, number, and stability are defined by such fundamental properties of the system as its *a priori* spatial-temporal symmetry as well as the nature of its approximate integral(s) of motion (its dynamical symmetry) and the topology of the corresponding reduced phase space. This is why the qualitative orbifold approach [1] guides the present study. The theory of invariants and the polynomial integrity basis (IB) construction become our major tools, indispensable both for the analysis of the normal form (the reduced Hamilton function) and for the orbifold construction. Thus, the use of the IB polynomials unifies the two approaches, algebraic and geometric.

The NNM's form the framework and the initial point for further dynamical study of the system. The two complementary ways of the analysis of the NNM's define the two major directions of this study. When the system is expected to exhibit substantially chaotic dynamics, the preference is given to the periodic orbit study. In this case it is often assumed that no approximate integrals of motion exist and a lot of work with numerical Poincaré surfaces of section to understand both the global dynamical structure on the phase space R_{2N} and the properties and bifurcations of individual periodic orbits follows.

At the same time, if certain approximate integrability is present in the system it would be very unwise to ignore it completely. Instead we should carefully analyze to what extent and at what perturbation levels we can trust our integrable approximation, the normal form, and at what point the structures on the phase space associated with integrability disappear. In doing so we apply the methods and ideology of the KAM theory. Finally, since our real systems are quantum we should transfer our results to the quantum analog of our classical problem. A few subjects of such research are closely related to the present paper and are discussed below.

A. Dynamical structure

As near any stable periodic orbit, the flow of the dynamical system in the vicinity of a stable nonlinear normal mode can be further reduced by the normal form methods [37]. The system near such orbit exhibits additional dynamical structure with the total action of the small oscillations about the orbit considered an approximate conserved quantity. The orbit itself lies at the center of this structure, both literally and figuratively—the structure is largely determined by such characteristics of the central orbit as stability and symmetry. Due to this latter fact such orbit is often called an "organizer" [38].

In the normal form approach of the present paper the motion along all central orbits is reduced simultaneously (as the motion with coordinate ϕ_n) and the period is defined for each orbit. We can now consider each stable relative equilibrium and further normalize near it. In fact, this work has been already commenced in Sec. IV E where the zero order (harmonic) Hamilton function for oscillations about those equilibria is derived. A more advanced study is presented in Ref. [8]. The complexity of the foliation of the reduced phase space depends on the resonances between different oscillatory modes (coiling oscillations about the orbit). In a simple case of reduced dimension two (one oscillatory mode) we find a system of 2D tori wrapped around the central orbit.

1. Invariant tori. Foliation of the C_s-invariant subspace

Reduction of the oscillatory problem near each relative equilibrium produces invariant tori T_2 on the reduced phase space $\Sigma = S_2 \times S_2$. These tori are in turn constant ϕ_n sections of the tori T_3 in the initial phase space R_6. The validity of the normal form approximation, or, in other words, the dynamical invariance of these T_3 tori can be investigated using appropriate Poincaré surfaces of section.

In the particular situation of the C_s-invariant subspace (the S_2 sphere) of Σ_4, invariant "tori" near the G_4 points are circles S_1, so that the tori in R_6 are of dimension 2 $[T_2 = S_1 \otimes S_1(\phi_n)]$. In the linear approximation the circles on the C_s-invariant sphere, and the action accumulated along them can be easily found from the position of of the G_4 points in Table III and the frequency ω in Table IV. Moreover, we can reconstruct the corresponding T_2 tori in the R_6 or take their projection on the configuration plane (ep) using the techniques described in Sec. IV D. In particular, propagating in phase ϕ_n, or moving along the invariant circle at constant ϕ_n we can reconstruct the sections of these tori. A qualitative study of such sections is discussed in Ref. [1].

2. Families of periodic orbits, orbits of higher periods

As in many other systems, periodic orbits of our problem can be unified in families. Each family begins with the central stable orbit, a "parent". Other orbits correspond to such oscillations about the central orbit whose period is commensurate with the period of the latter. (Thus orbits of period $k : l$ wind k times around the central orbit while passing l times along it.)

For all invariant tori discussed in the previous section our normal form methods can predict actions and periods of the motion along their principal directions and thus select the *resonant* tori. In other words, the normal form predicts the resonant tori filled with periodic orbits. It is well known, however, that the resonances between the motion along the central orbit and the oscillations about it *destroy* such tori (cf. Ref. [37]). In reality, instead of the resonant tori we only have their "skeleton" formed by one or, in the presence of symmetry—several isolated periodic orbits.

The above resonances are always present in the initial nonreduced system and are particular to each nonlinear normal mode. They cannot be taken into account by the simultaneous near-the-equilibrium reduction procedure of this paper. As a consequence, we can only find the tori on which the individual orbits in the family are lying, not the orbits themselves. Again, as a simple example we can study the destruction of the C_s resonant invariant tori T_2 near the G_4 orbits.

3. Chaotic dynamics and the validity of the normal form

The onset of chaotic dynamics begins with the destruction of resonant tori described in the previous section. Zones of irregular dynamics emerge around the destroyed tori. Stable periodic orbits remaining in place of these tori give rise to small stable islands and tori of their own. The structure within structure repeats. Nevertheless, as long as the volume of the phase space occupied by the zones of chaotic dynamics is small and these zones do not overlap we can continue to gather important dynamical information from the normal form.

Approaching the ionization threshold (at $S \approx 3/16$) is commonly associated with the complete breakdown of the normal form approximation and the truly chaotic dynamics. We have seen in Sec. IV C that the situation is not uniform: while the normal form definitely fails for (and near) the "downhill" G_4 orbit at $S = 0.18$, the two $\mathcal{T}_s$ orbits are reproduced with amazing accuracy. The "uphill" (small) G_4 orbit is also reproduced satisfactorily on the global scale, but the alternating formal series for its action and period converge very slowly in high orders.

This makes us believe that even at such high perturbations (energies) certain regular dynamical behavior still persists at least in some regions of the phase space and can still be traced back to the structure predicted by the normal form series. Moreover, we also conclude that for all nonlinear normal modes at the values of S up to 80% of the threshold value, the normal form prediction holds, and thus the regular dynamics should exist. The verification of this proposition requires further study of the dynamical structure and its manifestations by the normal form methods, as well as by the techniques commonly applied in chaotic systems, the periodic orbit methods, numerical Poincaré surfaces of section, and others.

B. Quantum-classical correspondence

As already mentioned above in Sec. II E, the normal form $H_{\text{n.f.}}$ as a function of n (and field strengths) has immediate semi-classical (EBK) interpretation. In the corresponding quantum system the action n is quantized, $n = 1, 2, 3, \ldots$. If the normal form series does not diverge the quantum multiplets of states with the same n, or *n-shells*, are well separated, and the $H_{\text{n.f.}}$ represents an effective Hamilton operator describing the internal structure of the shells. In particular, the value of $H_{\text{n.f.}}(n)$ (of energy) defined at the stable stationary (G_4-type) points gives the maximum and minimum energy, i.e., the splitting of the n-shell. Near each energy limit we observe regular sequences of quantum levels corresponding to a degenerate two dimensional quantum oscillator with harmonic frequency ω given in Table IV. The value of $H_{\text{n.f.}}(n)$ at the unstable ($\mathcal{T}_s$-type) points defines the transition region between the two systems of levels.

Like our reduction procedure, quantum mechanics also averages over the dynamical structure on the classical phase space. As a result, when the zone of classical chaos is small (in comparison with $\hbar$) we can still successfully apply the EBK quantization. This widely debated property of quantum systems adds an additional argument in favor of the normal form analysis of the presence of the integrable dynamics during the transition to chaos.

ACKNOWLEDGMENTS

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APPENDIX A: THE STUDY OF THE G_4 GROUP ACTION ON $S_2 \times S_2$

We use the realization of the four dimensional reduced phase space $\Sigma_4$as a subspace of the six dimensional Euclidean space with coordinates $(K_e, K_b, K_p; L_e, L_b, L_p)$. In other words, we consider points

$$s = (K_e, K_b, K_p; L_e, L_b, L_p) \in S_2 \times S_2, \tag{A1}$$

restricted by Eqs. (1) and (30) which define Σ_4.

1. The orbits of the group action

The action of the symmetry operations of the group G_4 on the points (A1) is given in Table I. Thus, for instance,

$$TC_2 : s \to (K_e, -K_b, -K_p; -L_e, L_b, L_p) \; . \tag{A2}$$

We first use Table I to find the *orbits* of the G_4 group action: we take one point on $S_2 \times S_2$ and find all other points which can be obtained from it by applying symmetry operations of G_4. The points in such orbit are related by symmetry transformations $\mathsf{R} \in G_4$ and are called *equivalent*. For each orbit we find its *stabilizer* $\mathfrak{g}$, a subgroup of G_4, whose operations map every point of the orbit onto itself. We also call $\mathfrak{g}$ the stability, the invariance, or the local symmetry group of of the orbit and of the corresponding points on $S_2 \times S_2$ [39]. Generic points form four-point orbits and have the trivial stabilizer C_1. In the general case of the finite total symmetry group $\mathfrak{G}$, the number of points in a generic orbit equals the number of the operations $[\mathfrak{G}]$, in our case $[G_4] = 4$.)

If some of the components of $\mathbf{K}$ and $\mathbf{L}$ equal zero we may obtain non-generic orbits with non-trivial stabilizers $\mathcal{T}_s$, C_s, $\mathcal{T}_2$ (Sec. I A 2), and even the whole G_4. Thus, the points

$$s' = (K_e, 0, 0; 0, L_b, L_p), \tag{A3}$$

are invariant with regard to TC_2 in (A2); they form two-point orbits because for both $\mathsf{R} = T\sigma^{(eb)}$ and $\sigma^{(ep)}$,

$$s' \xrightarrow{\mathsf{R}} (K_e, 0, 0; 0, L_b, -L_p) \xrightarrow{\mathsf{R}} s' \; . \tag{A4}$$

Required zero components for all possible stabilizers are given in Table II. In general for finite groups, the number of points in the orbit with stabilizer $\mathfrak{g} \subset \mathfrak{G}$ is given by $[\mathfrak{G}]/[\mathfrak{g}]$. In our example $[G_4]/[\mathcal{T}_2] = 2$. Each G_4 invariant point $(K_e, 0, 0; 0, L_b, 0)$ is itself an orbit of the G_4 group action, and the C_s, $\mathcal{T}_s$, and $\mathcal{T}_2$ invariant points form two point orbits.

2. Invariant manifolds

Invariant manifolds are subspaces of Σ mapped into itself by operations of $\mathfrak{g} \subset G_4$. The G_4 invariant manifold on Σ_4 is a circle S_1 defined by

$$K_b = K_p = L_e = L_p, \quad K_e^2 + L_b^2 = 1 \; . \tag{A5}$$

The $\sigma^{(ep)}$ invariant subspace is defined by

$$K_b = L_e = L_p = 0, \tag{A6a}$$
$$K_e^2 + K_p^2 + L_b^2 = \text{const}, \tag{A6b}$$

and Eqs. (1) defining Σ_4. All C_s invariant points form a two dimensional sphere S_2 with the points on the equator being of higher symmetry G_4 (cf. Sec. II C 1). The $\mathcal{T}_2$ invariant subspace is defined by

$$K_b = K_p = L_e = 0, \tag{A7a}$$
$$K_e^2 + L_b^2 + L_p^2 = \text{const}. \tag{A7b}$$

Similar to the C_s invariant manifold, the $\mathcal{T}_2$ manifold is a two-sphere S_2 whose equator is again the G_4 invariant circle. The $\mathcal{T}_s$ invariant subspace is defined by four equations

$$K_p = L_p = 0, \tag{A8a}$$
$$K_e^2 + K_b^2 + L_e^2 + L_b^2 = 1, \tag{A8b}$$
$$K_e L_e + K_b L_b = 0 \; ; \tag{A8c}$$

its geometry is more clearly seen if we rewrite these equations in terms of the components of $\mathbf{J}_1$ and $\mathbf{J}_2$ introduced in Eq. (31),

$$(J_1)_e^2 + (J_1)_b^2 = (L_e + K_e)^2 + (L_b + K_b)^2 = 1,$$
$$(J_2)_e^2 + (J_2)_b^2 = (L_e - K_e)^2 + (L_b - K_b)^2 = 1. \tag{A9}$$

Each of the Eqs. (A9) defines a circle S_1, so that the whole manifold is a two-dimensional torus T_2. This torus includes the G_4 invariant circle ($K_b = L_e = 0$). All other points on the torus (with $K_b^2 + L_e^2 \neq 0$) form two point orbits $(K_b, L_e, \pm K_b, \pm L_e)$.

3. Stratification

We remind the difference between the decomposition of the manifold into strata, often used in the study of group actions on manifolds [15], and into invariant subspaces introduced in Sec. A 2. In brief, an invariant manifold can contain several strata.

Group orbits are said to be of the same type if their stabilizers are the same. Orbits of the same type form a stratum; two points of the manifold belong to the same stratum if and only if their stabilizers are the same [39].

Zero-dimensional strata are invariant subspaces. Strata of higher dimension constitute invariant manifolds only if they are *closed*. Open strata, such as the generic stratum, which is always open and dense, form invariant manifolds together with their closure. Resulting manifolds include several strata simultaneously. Thus the G_4 stratum is an invariant manifold S_1, while the C_s manifold S_2 consists of the G_4 and C_s strata.

The gradients of all invariant functions vanish on the orbits which are *isolated* in their strata. These orbits are often called *critical* [15]. In particular, orbits on zero-dimensional strata are always critical. Critical orbits exist in the hydrogen atom problem in the Zeeman and Stark limits, or in the case of two parallel fields [2,3]. No critical orbits exist in the case of two orthogonal fields. Positions of stationary points are not fixed within the strata. To get restrictions on the number of stationary points on different strata and invariant manifolds we apply Morse theory [32,33] in Sec. III C.

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[12] It should be understood that the choice of scaled field constants is not universal. Many authors tend to use quadratic Zeeman effect as the initial point of their study. They use scaled electric field parameters F_s of the type FG^{-2} [28] or $FG^{-4/3}$ [6], so that the Stark limit lies at $F_s \to \infty$ and this clearly implies *small* electric fields. Thus, for instance, the collapse phenomenon [3] has long remained unnoticed due to such traditional parameterization.

[13] The terms in the generator of $\mathfrak{L}$ "replicate" the nonresonance terms of the Hamilton function [30] and in most cases the symmetry of the latter is preserved automatically; in particular, $\mathfrak{L}$ commutes with operations in G_4.

[14] The study of the group action on the phase space is an important initial step of the symmetry analysis. In this work we use the results of this step to take into account the finite symmetry G_4. For an introduction to the treatment of dynamical systems with symmetries see J. E. Marsden and T. S. Ratiu, *Introduction to Mechanics and Symmetry* (Springer, New York,1994) and references therein.

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[17] Enlargement has many applications in physics and mathematics. We mention two very different physical problems. The Calogero system of N particles on a line with an inverse square potential, a system with $2N$-dimensional phase space, can be considered as the reduction of a very simple Hamiltonian flow on a $2N^2$-dimensional phase space; the quasicrystals can be interpreted as periodic structures in higher dimensions.

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