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 parametrization 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 eight-dimensional space and then reduced explicitly to the $S_2\times S_2$ reduced space of the n shell using the Lie transformation to the third order in S. At fixed S the system is uniformly tuned between the Zeeman and the Stark limits using the analytic formulas of the perturbation theory. The approach requires application of the invariant theory, group theory, and topology to the 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 $S_2\times S_2$. [S1050-2947(98)01404-8]

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I. INTRODUCTION

The hydrogen atom in the presence of static external fields is a fundamental, relatively simple problem with many different kinds of dynamical behavior. It has become a test ground for the dynamical system analysis, semiclassical theory, and a number of modern experimental techniques that provide highly accurate data on the actual quantum system.

In the present paper we focus on the hydrogen atom in orthogonal (crossed) electric and magnetic fields [1]. (See Sec. I A for a precise definition and notation.) The dynamics of this system with three degrees of freedom can be very complex and it is natural to begin with the nearly integrable case at relatively small fields and to study changes in its dynamical structure caused by increasing perturbation.

Our main object is the four families of principal periodic orbits, the nonlinear normal modes of the crossed-field problem, and the corresponding relative equilibria [2]. In this regard we should pay tribute to the two earlier papers by Flöthmann *et al.* [3] and by Uzer and co-workers [4,5]. In Ref. [3] the authors initiated 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. [4,5] rely essentially on the second-order perturbation theory and the dynamical analysis of the reduced Hamilton function of the problem. We follow this work using more extensively the methods of qualitative dynamics, topology, and group theory [6–8].

The unperturbed hydrogen atom is an integrable system with continuous spatial symmetry O(3) and dynamical symmetry O(4); 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, $E=-1/2n^2$. We consider n, the principal Coulomb integral, as an approximate integral of motion of the atom-in-field problems. The quantum analog of n is of course the principal quantum number n. This so-called n-shell model is explained further in Sec. II C.

Instead of analyzing our problem directly on the initial six-dimensional phase space R_6, we first use approximate integrability to reduce R_6 to the space Σ_4 of dimension 4, analyze the dynamics there, and use the correspondence between the reduced and the initial problems. This central dynamical idea of our paper is explained in Sec. I B.

A. Hydrogen atom in crossed fields

We introduce the notation and the Hamilton function, find the symmetry group, and define the parametrization required for a uniform representation of all orthogonal field configurations and convenient ''tuning'' between the Zeeman and Stark limits [9].

1. Hamilton function

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

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

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

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

2. Symmetry group

Our Hamilton function (3) is invariant with regard to three nontrivial discrete spatial-temporal symmetry operations R [6]: $\sigma^{(ep)}$ is the reflection in the plane orthogonal to **G**, $T\sigma^{(eb)}$ is a combination of time reversal $(q,p)\rightarrow(q,-p)$ and reflection in the plane spanned by **G** and **F**, and TC_2 is the combination of the time reversal and rotation by π around axis **F**. Together with identity I these operations form an order-4 group G_4, the total symmetry group of the crossed-field problem, with three order-2 subgroups.

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

3. Parametrization

We want to study the dynamics of the problem for *all* ratios of the two field strengths while the total effect of the perturbation is kept more or less the same [9] and our parametrization differs from that used elsewhere [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 $\approx\pm 3Fn^4$ with $n\approx\sqrt{-1/2E}$. Then for given n it is natural to fix

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

and to vary only the relative strengths of the two fields

$$G_s=Gn^3/S, \quad F_s=3Fn^4/S. \tag{4b}$$

In this paper we consider small values of S and *all* possible relative strengths of the two fields, such as

$$F_s=\cos\alpha, \quad G_s=\sin\alpha, \quad 0\leqslant\alpha\leqslant\frac{\pi}{2}. \tag{4c}$$

B. Correspondence between the reduced and the initial phase spaces

Our use of n in Eq. (1) as an *approximate* integral is quite typical: In a physical problem with N degrees of freedom and the phase space R_{2N}, 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. 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 $Q=P=0$,

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

whose zeroth-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 and eliminate all terms h in H_k with $\{h,H_0\}\neq 0$ by an appropriate canonical transformation.

The resulting Hamilton function of the reduced problem is called the *normal form* H_{NF}. The normal-form transformation is a canonical near identity change of variables $\mathfrak{L}$ that maps the original phase space R_{2N} onto a space of the same dimension (and topology) $\mathcal{R}_{2N}$,

$$R_{2N}\overset{\mathfrak{L}}{\rightarrow}\mathcal{R}_{2N}\mapsto\Sigma_{2N-2}. \tag{6}$$

The normal form $H_{\rm NF}$ defined on $\mathcal{R}_{2N}$ 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 $H_{\rm NF}$ no longer depends on ϕ_n). For fixed n we consider $H_{\rm NF}$ as a Hamilton function defined on a *reduced* phase space Σ of dimension $2N-2$.

$H_{\rm NF}$ is obtained as a formal power series and generically is divergent. Physically it is clear that we cannot equivalently replace the original nonintegrable system by an integrable one. Nevertheless, we can still understand many important global features of this original system using $H_{\rm NF}$. To actually use Σ in the analysis we *truncate* $H_{\rm NF}$ and thus assume that n is a strict integral of motion. The extent to which we represent the original dynamics 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} and the initial phase space R_{2N} is in their global properties: while R_{2N} is a simple Euclidean space (with a symplectic structure $dq\wedge dp$), the topology of and the symplectic structure on Σ_{2N-2} depend on the nature of the approximate integral n, i.e., on the approximate dynamical symmetry we assume. They can be quite complex. In our case [10] $N=3$ and the original phase space is R_6, n is defined by Eq. (1), and the four-dimensional reduced phase space Σ_4 is the direct product of two spheres $S_2\times S_2$ (Sec. II C). The global aspect of the dynamical structure on Σ_{2N-2} is entirely defined by the topology of Σ: Due to the nature of the approximate integral n, the dynamics of a particular reduced problem will have certain common features.

3. Dynamical structure on Σ and on R

Assuming 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 Γ of the reduced space Σ, the image of Γ in $\mathcal{R}$ is a product of Γ and a circular orbit S_1 defined by ϕ_n, $\Gamma\otimes S_1(\phi_n)$. To obtain the image in the original phase space R we use $\mathfrak{L}^{-1}:\mathcal{R}\rightarrow R$ [cf. Eq. (6)]. Thus stationary points [2] 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) is invariant with respect to all operations R of the group G_4 in Sec.

I A 2. These operations act on the initial phase space $R_6(Q,P)$ and thus on any function defined on it. By construction, our normal form transformation $\mathfrak{L}$ preserves the G_4 symmetry [13] and so $H_{\rm NF}$ inherits this symmetry from the initial Hamilton function (3).

We study the *action* of the operations R of G_4 on the phase space and on other dynamical objects such as vector fields, flows, and periodic orbits [14]. The phase space is subdivided into *strata*, or sets of points with different symmetry properties [15]. Strata of dimension zero, i.e., sets of isolated points, are of particular interest since they necessarily correspond to the stationary points [2] of any smooth G_4-invariant Hamilton function. We also distinguish invariant subspaces that 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 the Appendix. 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 (Sec. III).

1. Spatial symmetry

In the simplest case we have *linear symplectic* operations R, which are easily applied to any of the above objects; the operation

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

is an example. The main consequence of this spatial symmetry is the existence of a dynamically invariant subspace of the phase space R_6. Indeed, the equation $Q_b=P_b=0$ defines a subspace R_4 of R_6, that is both invariant with regard to C_s, the group generated by $\sigma^{(ep)}$, and dynamically invariant: Any trajectory with initial conditions $Q_b=P_b=0$ remains in this subspace, i.e., the electron will move in the plane (e,p) orthogonal to the magnetic field vector **G**. Two major periodic orbits of the entire problem lie in this plane and can therefore be studied more easily using the C_s-restricted Hamilton function.

2. Spatial-temporal symmetry

Operations of G_4 involving time reversal T require more attention. These operations cannot be adequately represented on the phase space. Formally, their action can still be defined. This action is not symplectic, does not preserve the Hamiltonian flow (does not commute with this flow), and can only be used for the analysis of stationary points [2].

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

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

can be formally given by a nonsymplectic operation

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

and as such can be applied to the 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. However, except for the stationary points, any structure that exists on the phase space due to Eq. (8b) is irrelevant to the behavior of the flow of the dynamical system (Sec. III B).

3. Nonlinear action and dynamical symmetry

Our situation is more complex because the total symmetry group O(4), exact for the unperturbed hydrogen atom and approximate for the whole problem, has *nonlinear* action on the initial phase space R_6. This symmetry is dynamical and its operations commute with the flow of the unperturbed problem. We *linearize* the action of this dynamical group by changing to a space of higher dimension (Sec. II A) where the ϕ_n flow of the whole problem is made *perfectly* linear by the normal form transformation. Once linearized, all symmetry operations of the problem are easily combined and analyzed.

II. REDUCED PROBLEM FOR CROSSED FIELDS

A. Reduction or enlargement?

In the process of reduction the dynamical flow of the perturbed problem corresponding to the approximate integral n is linearized and all points that differ only in phase ϕ_n (orbits of n) are mapped onto one point of the reduced space Σ. Such a procedure is regarded traditionally as ''simplification'' since the number of variables is reduced. At the same time, the flow on Σ naturally becomes more complicated.

The procedure of 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. If this is not the case, we can linearize this group action 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.

Our initial phase space is R_6. To linearize the action of O(4) we enlarge the dimension by 2. The actual transition $R_6\rightarrow R_8$ 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 that differ only in the value of the conjugated angle ϕ_ζ.

Another important reason for the KS transformation is the *regularization* of the $1/r$ Coulomb potential [20]. Indeed, our normal form reduction (Sec. I B 1) works only if the Hamilton function H is regular near the equilibrium $Q=P=0$ [cf. Eq. (5)]. In the KS coordinates the function (3) is regularized by taking $H\rightarrow Hr$ ($t\rightarrow t/r$ for time) and the problem transforms into a special four-dimensional oscillator.

B. KS transformation and regularization

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

$$M_{\rm KS}=\begin{pmatrix} q_1 & -q_2 & -q_3 & q_4 \\ q_2 & q_1 & -q_4 & -q_3 \\ q_3 & q_4 & q_1 & q_2 \\ q_4 & -q_3 & q_2 & -q_1, \end{pmatrix} \qquad (9)$$

with q the coordinates in R_4. The coordinates (Q_1,Q_2,Q_3) in the physical space R_3 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 $Q_4\equiv 0$. The radius in R_3 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 $M_{\mathrm{KS}}^T M_{\mathrm{KS}}=M_{\mathrm{KS}}M_{\mathrm{KS}}^T=rI_4$. 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 the factor $1/r$, the *same* as in the Coulomb potential. The KS transformation defined by Eqs. (10) and (11) is canonical. However, for P_4 in Eqs. (11) to become identically zero we impose the restriction

$$\zeta\overset{\mathrm{def}}{=}-2rP_4=q_1p_4-q_4p_1+q_3p_2-q_2p_3=0. \tag{12}$$

Thus the initial phase space $R_6=\{Q_1,Q_2,Q_3,P_1,P_2,P_3\}$ of the Kepler and Coulomb problems becomes a reduced space for a problem in $R_8=\{q_1,q_2,q_3,q_4,p_1,p_2,p_3,p_4\}$ with the integral $\zeta=0$ [21].

Using the KS formulas (10) and (11) together with condition (12), we find the three-dimensional space 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 terms of R_8:

$$L_b=\tfrac{1}{2}(q_1p_4-q_4p_1+q_2p_3-q_3p_2)$$
$$=q_2p_3-q_3p_2, \tag{14a}$$

$$L_e=\tfrac{1}{2}(q_2p_4+q_3p_1-q_1p_3-q_4p_2), \tag{14b}$$

$$L_p=\tfrac{1}{2}(q_1p_2+q_3p_4-q_2p_1-q_4p_3), \tag{14c}$$

where $(1,2,3)=(e,b,p)$ [Eq. (3) and Sec. I].

1. Hamilton function in KS coordinates

We use Eqs. (10), (11b), and (14a) to express $H(P,Q)$ in Eq. (3) in terms of (q,p) in R_8,

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

with E the energy. Equation (15a) multiplied by $4r$ becomes regular,

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

The new Hamilton function is a polynomial in (q,p),

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

whose quadratic part represents an isotropic harmonic four-oscillator with frequency

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

Scaled to the standard form by

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

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

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

The harmonic part of the oscillator (18) is the total action proportional to the principal integral of motion n of the unperturbed Coulomb problem [Eq. (1)]. Since $4/\omega=2n$ [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. Eq. (21) and Eq. (22) of Ref. [22], and Ref. [23]],

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

Substitution of the KS formulas into Eqs. (10), (11), and (14) yields complicated expressions that, however, can be radically simplified using $\zeta=0$ [Eq. (12)] and our assumption $n=\mathrm{const}$ that restricts Eq. (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 $K\rightarrow 2K$ 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 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.

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 $n_i=\frac{1}{2}(q_i'^2+p_i'^2)$, $i=1,\ldots,4$.

Because of 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 $z_i=q_i'\pm ip_i'$ coordinates, the operation $\{,\zeta\}$ maps each individual monomial $h=z_1^{a_1}\cdots z_4^{a_4}\bar{z}_1^{b_1}\cdots\bar{z}_4^{b_4}$ 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 $a_1+\cdots+a_4+b_1+\cdots+b_4$). 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. [4] for further details.

4. Restriction on the C_s-invariant subspace

As already pointed out in Sec. I C 1, the spatial symmetry group of our problem is C_s. To study 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 $\sigma^{(ep)}$,

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

and one corresponding invariant subspace in R_8 with

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

TABLE I. Transformation properties of the dynamic variables of the n-shell reduced problem under the action of G_4.

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

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

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

$$\widetilde{H}=p_2^2+q_2^2+p_4^2+q_4^2+\frac{2}{3}(q_2^4-q_4^4)f+(q_2+q_4)\times(q_2p_4-q_4p_2)g+\frac{1}{4}(q_2^2+q_4^2)^3g^2=\frac{4}{\omega}. \tag{27}$$

Like the motion in the (e,p) plane of the initial physical space, the C_s-restricted problem in the KS coordinates has two degrees of freedom.

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

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

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

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

$$\widetilde{L}_b=q_2p_4-q_4p_2, \tag{29b}$$

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

$$\widetilde{K}_p=-q_2q_4-p_2p_4. \tag{29d}$$

C. Reduced phase space $S_2\times S_2$

Reduction with regard to n is realized in the KS space R_8 as a standard Lie transformation [Eq. (6)]; reduced space Σ_4 is obtained from the transformed space $\mathcal{R}_8$ using *both* $n=\text{const}$ and $\zeta=0$. Since our H_{NF} is truncated and n is assumed to be strictly conserved, the phase space Σ_4 is the same as for the unperturbed hydrogen atom. We use the components of L and K with two restrictions (1) as dynamical coordinates on Σ_4 and take advantage of the $n=\text{const}$ condition to introduce universally scaled vectors,

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

In other words, we project all n shells on the shell $n=1$ and scale all KS coordinates in $\mathcal{R}_8$ by the hyperradius $\sqrt{n}$,

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

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 conclude that Σ_4 is a direct product of two two-dimensional spaces. Furthermore, since each $\mathbf{J}_i$ has the properties of an angular momentum $\{J_{ie},J_{ib}\}=J_{ip}$ and the magnitude of each $\mathbf{J}_i$ is fixed, Σ_4 is a direct product of two spheres $\Sigma_4=S_2\times S_2$. The important implications of this topology are explained in Sec. III C.

1. Reduced phase space of the C_s-restricted problem

Reduction of the C_s-restricted problem (27) is similar to that of many other two-oscillator problems. It is made near $q=0$ with regard to the combined action $\widetilde{n}$ in Eq. (29). The reduced phase space, a two-sphere S_2 (isomorphic to the complex projective space CP_1), is the C_s-invariant subspace of the reduced space Σ_4 (Sec. III A).

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

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

In fact, expressions for $(\widetilde{L}_b,\widetilde{K}_e,\widetilde{K}_p)$ in Eq. (29) give the standard construction of the angular momentum vector $\mathbf{J}=2\mathbf{J}_1$ (with $\widetilde{K}_e$ usually regarded as J_z) in terms of the coordinates of an isotropic two-oscillator [25].

D. Symmetry properties and integrity basis

We 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 $\mathbf{L}=(L_e,L_b,L_p)$. Transformation properties of these variables are summarized in Table I. They can be verified directly from the definition of the action of the G_4 group on the initial space Σ_6, such as in Eq. (7), by inducing their action on Σ_8 and applying it to the KS definitions (14) and (22).

Using symmetry properties and the basic theory of invariants, we construct the set of G_4-invariant polynomials, or the *integrity basis* (IB). These polynomials have two important properties: (i) They are necessary and sufficient to represent a polynomial (power series) expansion of any G_4-invariant function on $\Sigma=S_2\times S_2$, such as $H_{\rm NF}$ and (ii) the values of these polynomials label uniquely the orbits of the action of the G_4 group on Σ.

1. Construction of the integrity basis

The space $\Sigma_4=S_2\times S_2$ has dimension four and the IB includes four main invariants. For G_4 acting on Σ_4 it also includes three auxiliary invariants. The theory specifies their construction as follows.

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 IB is ambiguous. We take

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

as basic invariant polynomials and

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

as auxiliary.

2. IB for the C_s-restricted problem

The C_s-restricted problem has a very simple IB: Its reduced phase space S_2 (Sec. II C 1) is of dimension 2 and the two main invariants are naturally $\widetilde{K}_e$ and $\widetilde{L}_b$ 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 [cf. Eq. (28)]. The remaining $\widetilde{L}_p^2-\widetilde{K}_p^2$ is not needed because it depends linearly on $\widetilde{K}_e^2$ and $\widetilde{L}_b^2$ [cf. Eq. (33)]. The absence of auxiliary invariants is due to the fact that G_4 acts on the (L_b,K_e,K_p) space as an order-2 reflection group (cf. Table II) and the IB for groups generated entirely by reflections contains no auxiliary invariants [26].

3. Application of IB polynomials

We can now represent any G_4-invariant polynomial on Σ using the IB polynomials (34) 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

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

and $c^i,c^i_{2a},c^i_{2b},c^i_4$ numerical coefficients. On the other hand, IB polynomials (34a) serve as correctly defined coordinates on the space of group orbits of G_4, the orbifold [26].

E. Parametrization of formal series

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

To construct these series we choose the 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 $x=(q_1,\ldots,q_4;p_1,\ldots,p_4)$. Generally, factors g

TABLE II. 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 oder
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	$-S^2F_s^2(3G_s^2-2)/36$	

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

and f in Eq. (18) suit this purpose: If they are both assumed to be of order τ, i.e., $g \sim \tau$ and $f \sim \tau$, then $H(x) \sim x^2(1 + \tau x^2 + \tau^2 x^4 + \cdots)$.

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

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

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 so there is no point in any rigorous discussion of the convergence and we simply truncate our series. 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 formulas should apply only below such a 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

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

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

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

where r is 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 Eqs. (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 left-hand side of Eq. (40c),

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

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

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

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 $S<3/16$. We can see from Eq. (37) 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. (This is generally known as the possibility to scale our classical problem.) We also note that Eq. (42a) is a static estimate of $S_{\rm crit}$ and no similar dynamical limitation can be suggested until we define quantitatively which features of the dynamics we want to be reproduced by our normal form and how precise this reproduction should be (see Sec. V A 3).

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 [27] $R_8(x)\overset{\mathfrak{L}}{\to}\mathcal{R}_8(y)$. The nonlinear near-identity transformation $\mathfrak{L}$ and the inverse $\mathfrak{L}^{-1}$ are obtained explicitly as formal Taylor series. 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 [28].

To represent the resulting normal form $H_{\rm NF}$ we use the n-scaled $\mathbf{K},\mathbf{L}$ coordinates (30a) of Sec. II C, such that

$$H_{\rm NF}=4/\omega, \tag{43a}$$

$$H_{\rm NF}=2n\left(1+\frac{\tau}{2}H_1+\frac{\tau^2}{4}H_2+\frac{\tau^3}{2^5}H_3+\cdots\right), \tag{43b}$$

where, except for the overall unperturbed energy factor $2n$, all explicit n dependence is absorbed in the formal parameter τ [Eq. (38)] and in the scaled normalized field strengths F_s and G_s [Eq. (39)]. Since $H_{\rm NF}$ is G_4 invariant (Sec. I C), all resonance terms H_k can be expressed in terms of the G_4-invariant polynomials in Sec. II D,

$$H_1=G_sL_b-F_sK_e, \tag{44a}$$

$$H_2=-[3L_b^2-2K_e^2+3K_b^2+2L_e^2+2(L_p^2-K_p^2)-3]G_s^2/4+(7K_eL_b-L_eK_b)F_sG_s/3-(51K_e^2-9L_e^2+17)F_s^2/36, \tag{44b}$$

$$H_3=L_b(6L_e^2-6K_e^2+9K_b^2+5L_b^2+6(L_p^2-K_p^2)-9)G_s^3-K_e(125-43L_e^2+125K_e^2)F_s^3/9$$
$$+[-45K_eL_e^2+45K_e^3-65K_eK_b^2+117K_e-147L_b^2K_e-45K_e(L_p^2-K_p^2)+48L_b(L_eK_b)]F_sG_s^2/6$$
$$-[3K_b^2L_b+87L_e^2L_b-615K_e^2L_b-3L_b^3-232L_b-3L_b(L_p^2-K_p^2)+108K_e(L_eK_b)]F_s^2G_s/18. \tag{44c}$$

Note that in order to obtain the above formulas 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 can we set $\zeta=0$.

The procedure to obtain the C_s-restricted normal form of Eq. (27) is the same, but the calculation is much simpler. The resulting $\widetilde{H}_{\rm NF}$ depends only on $\widetilde{n}$, $\widetilde{K}_e$, and $\widetilde{L}_b$ in Eqs. (29), and ζ is not involved since $\zeta\equiv0$. The lower orders equal those in Eqs. (44) restricted using Eqs. (28) and (33). The fourth-order contribution is $\tau^4 2^{-7}\widetilde{H}_4$ with

$$\widetilde{H}_4=-\frac{17\,815}{216}F_s^4\widetilde{K}_e{}^4+\frac{2468}{9}G_s\widetilde{L}_bF_s^3\widetilde{K}_e{}^3-\frac{39\,685}{108}G_s^2\widetilde{L}_b{}^2F_s^2\widetilde{K}_e{}^2+\frac{2047G_s^2+49}{9}G_s\widetilde{L}_b{}^3F_s\widetilde{K}_e-\frac{368+3853G_s^2}{72}G_s^2\widetilde{L}_b{}^4$$
$$+\frac{48\,218G_s^2-17\,815}{108}F_s^2\widetilde{K}_e{}^2-\frac{17\,297G_s^2-7886}{27}G_s\widetilde{L}_bF_s\widetilde{K}_e+\frac{27\,152G_s^2-13\,787}{108}G_s^2\widetilde{L}_b{}^2-\frac{2095}{18}G_s^4+\frac{4523}{54}G_s^2-\frac{3563}{216}. \tag{45}$$

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

Two factors, the geometry of the reduced phase space Σ and the symmetry G_4, result in certain important generic features of any Hamilton function $H_{\rm NF}$ on Σ [6]. These general properties are universal; they can be established without any particular (analytic) form of the function $H_{\rm NF}$ [such as in Eqs. (43a) and (44)].

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

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

The $S_2\times S_2$ itself consists of ''mostly'' generic points and thus can be considered as a C_1-invariant manifold that 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. The G_4-invariant (the fourth) submanifold is necessarily the intersection of the three.

Table III summarizes the algebraic description of these invariant submanifolds. We list the components of **K** and **L** that must vanish to satisfy the particular local symmetry (cf. Table I) and then simplify general equations (30) defining the whole $S_2\times S_2$ in $R_6(\mathbf{K},\mathbf{L})$ (last column in Table III). These simplified equations demonstrate the topology of submanifolds: the set of G_4 invariant points is a circle S_1; the C_s and $\mathcal{T}_2$ invariant manifolds are spheres S_2; the $\mathcal{T}_s$ invariant subspace is a two-dimensional torus whose two principal circles can be represented by the e and b components of $\mathbf{J}_1$ and $\mathbf{J}_2$ [cf. Eq. (31)]. We can easily see from Table III that the G_4 circle is indeed the intersection of the C_s, $\mathcal{T}_s$, and $\mathcal{T}_2$ submanifolds.

B. Special role of time reversal

We must distinguish invariant manifolds with purely spatial stabilizers $\mathfrak{g}$ from those whose stabilizers include reversing-symmetry operations $T\sigma$ and TC_2 in Sec. I A 2. All invariant submanifolds are equally important for the analysis of relative equilibria [2]. To simplify the search for the stationary points we can restrict $H_{\rm NF}$ on any of the invariant submanifolds. If a point is found, it will automatically be stationary for the $H_{\rm NF}$ on the whole of Σ. (The gradient of $H_{\rm NF}$ in the direction orthogonal to the invariant submanifold vanishes.) Special symmetry properties of such a stationary point mean special symmetry properties of the corresponding periodic orbit (cf. Sec. I B 3 and see Sec. IV).

At the same time, classical trajectories or, more generally, the flux of $H_{\rm NF}$ on the reduced phase space Σ, respect only a purely spatial invariance and we can restrict the flux of the $H_{\rm NF}$ to a submanifold of Σ if $\mathfrak{g}$ is purely spatial because the vector field is tangential to such submanifold and all classical trajectories remain on it. It follows that we can study independently the set of C_s-invariant trajectories together with G_4-invariant trajectories as their subset. (The flux is tangent to the C_s invariant sphere $S_2\subset\Sigma$ and to its ''equator,'' the G_4-invariant circle $S_1\subset S_2$.)

C. Stationary points of $H_{\rm NF}$ on Σ

Relations between the topology of the manifold and the system of stationary points of a smooth function $H_{\rm NF}$ defined on it is the subject of Morse theory [29]. In particular, any smooth Morse-type function $H_{\rm NF}$ 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).

Since G_4 is a finite group, it is natural to suppose that all stationary points of a generic G_4-invariant function $H_{\rm NF}$ defined on $\Sigma=S_2\times S_2$ are isolated and nondegenerate [30]. We consider and combine the topological restrictions on the stationary points of $H_{\rm NF}$ for all manifolds listed in Table III. The minimum number and the type of stationary points required by the Morse theory for each of these manifolds individually is as follows.

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

In the presence of the G_4 symmetry, the minimum number of stationary points is 4: All requirements of the Morse theory for each of the four submanifolds 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 onto each other by operations TC_2 or $\sigma^{(ep)}$ that 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 the Appendix.)

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. 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 $\nu K_e+\mu L_b$ (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 (see Sec. IV A 1). The situation might be more complicated in the limit $\mu=0$ or $\nu=0$ and might depend on the quadratic terms.

The position of stationary points on their respective invariant submanifolds is not defined by symmetry. (The group orbits formed by these points are not isolated within their strata; see Sec. 2 of the Appendix). When the parameters of the $H_{\rm NF}$, 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 than 4 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_{NF} [31].

IV. NONLINEAR NORMAL MODES DERIVED FROM THE REDUCED PROBLEM

The four principal relative equilibria [2] of the generic G_4-invariant function H_{NF} over the reduced phase space $S_2 \times S_2$ (Sec. III C) correspond to four principal families of periodic orbits of the original problem (cf. Sec. I B) so that the symmetry properties and stability of the orbits can be deduced from the characteristics of the stationary points. Furthermore, the action along the orbits and the period can be derived from the normal form in Eqs. (43b) and (44) and even the initial physical phase-space image of the orbits can be reconstructed from the position of stationary points on Σ and the explicit transformation formula (6). The four relative equilibria exist at all possible values of field parameters and only they exist at infinitesimally small (but nonzero) parameters. The corresponding four families of periodic orbits possess, of course, the same property and we call them nonlinear normal modes.

A. Evolution between the Zeeman and Stark limits

To have a general idea of what happens to the four nonlinear normal modes when the field configuration changes from the Zeeman to the Stark limit, we analyze the behavior of the corresponding four stationary points in the lowest-order approximation (cf. Ref. [3]).

1. Linear approximation

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

$$H_{\mathrm{NF}}=2n\left[1+\frac{\tau}{2}(G_sL_b-F_sK_e)+\cdots\right]=\frac{4}{\omega}, \qquad (46)$$

find its four stationary points on $S_2\times S_2$ using Eqs. (1) and (30a), and characterize the points in terms of IB polynomials (34).

$\mathfrak{g}$	K_e	Kb^2	Le^2	L_b	$K_p^2-L_p^2$	H_{NF}
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 form one orbit of the G_4 group action) the values of invariant polynomials and therefore all G_4-invariant characteristics of these two points including the value of H_{NF} will be the *same* (to any order in τ). On the contrary, the two G_4-invariant points are not equivalent.

As expected in Sec. III C, the stationary points of H_{NF} 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_{NF} (for the same n shell, $n=\mathrm{const}$). The two $\mathcal{T}_s$-symmetric stationary points remain unstable. Such monotone evolution of the stationary points between the two limits is very different from the case of the two parallel fields [6,7].

2. Properties of nonlinear normal modes

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. Since each stationary point has one nonzero component of the orbital momentum **L**, all corresponding periodic orbits are loops in the initial physical configuration space R_3 (as opposed to lines that run in both directions). From the linear solution (Sec. IV A 1) we can see that the G_4-type orbits loop around axis b ($L_b\neq 0$), while the $\mathcal{T}_s$-type orbits loop mainly around axis e ($L_e\neq 0$). Since G_4 contains no time reversal, all these loops in R_3 have one distinct direction.

The G_4-invariant trajectories must lie in the (e,p) 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 III). 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); in particular, they are not parallel to the (b,p) plane. The two $\mathcal{T}_s$ trajectories are equivalent: The operations $\sigma^{(ep)}$ and TC_2 map them onto each other.

3. Symmetry of the Zeeman and Stark limits

The symmetry of the two limits is much higher than G_4 [6]; 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 and in addition to simple stationary points, generic functions on $S_2\times S_2$ in the presence of such symmetry can possess stationary (critical) manifolds S_1 [30]. Our four principal relative equilibria remain simple nondegenerate stationary points in both limits.

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 lie in the

(ep) plane (orthogonal to the field axis) and run in two different directions along two circles with different radii (see Fig. 2 later in Sec. IV D).

In the Stark limit, the same two G_4 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. The ''downhill'' trajectory is longer than the ''uphill'' 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 action of the G_4 symmetry group. 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 in Sec. IV D). The two lines are equivalent; the $\sigma_h=\sigma^{(ep)}$ operation maps them onto 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 ($Q_e=\text{const}\neq 0$; 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 a separate detailed analysis.

B. Position of stationary points

We know from the linear solution in Sec. IV A 1 that the position of the four relative equilibria on Σ depends on the parameters F and G and we can express it as a formal power series. The order of the series is limited by the order 3 to which the normal form in Eqs. (43a), (43b), and (44) is developed.

1. Choice of formal parameter

Periodic orbits of nonintegrable systems are studied at given fixed energy $E=\text{const}$. In the presence of the approximate integral n the energy remains a preferred parameter when an exact (numerical) orbit is sought or when the n-shell approximation is expected to break in the transition-to-chaos region. Consequently, we take 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 (43b) 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 is valid only if n can be regarded as an integral of motion and therefore 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). Another advantage of having n as an independent parameter in the reduced problem is the possibility of applying directly the semiclassical Einstein-Brillouin-Keller (EBK) quantization. When we use either n (or τ) or E (or S) as an independent parameter (in addition to the field strengths G and F), we should be able 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. Value of n as a function of energy and field strengths

The principal integral of motion n as a 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

$$H_{\mathrm{NF}}(\mathbf{K},\mathbf{L};n,\tau,F_s,G_s)=\frac{4}{\omega(E)}=\text{const}. \tag{47}$$

Remember that we use normalized vectors $\mathbf{K}$ and $\mathbf{L}$ [Eq. (30a)] and all dependence of the H_{NF} in Eq. (47) [in Eqs. (43a) and (44)] on n is concentrated in the parameter τ. To solve (reverse) Eq. (47) as a formal power series in S, we multiply Eq. (43b) by $\frac{1}{4}S\omega$ so that

$$S=\tau+\frac{\tau^2}{2}H_1+\frac{\tau^3}{4}H_2+\frac{\tau^4}{32}H_3+\cdots, \tag{48a}$$

and consequently

$$\tau=S-\frac{S^2}{2}H_1+\frac{S^3}{4}(2H_1^2-H_2)-\frac{S^4}{32}[20H_1(H_1^2-H_2)+H_3]+\cdots, \tag{48b}$$

with functions H_k given by Eqs. (44) above. From Eq. (38) we see immediately that

$$n=\frac{2}{\omega}\left[1-\frac{S}{2}H_1+\frac{S^2}{4}(2H_1^2-H_2)+\cdots\right]. \tag{48c}$$

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 relative equilibria in Sec. III C we look for the extrema of either the normal form $H_{\mathrm{NF}}(\mathbf{K},\mathbf{L};\tau,n,G_s,F_s)$ in Eqs. (43b) and (44), i.e., the energy E, or the value of $n(\mathbf{L},\mathbf{K};E,G,F)$ in Eq. (48c). In either case the coordinates $(L_e,L_b,L_p,K_e,K_b,K_p)$ of the stationary points obey the system of conditional extremum equations

$$\nabla_{\mathbf{K},\mathbf{L}}\Phi=0,\quad \mathbf{K}^2+\mathbf{L}^2=1,\quad \mathbf{K}\cdot\mathbf{L}=0. \tag{49}$$

with $\Phi=H_{\mathrm{NF}}$ or n, and restrictions (30) imposed on the six components of the gradient by the $S_2\times S_2$ topology. The formal series solutions to Eqs. (49) are obtained by Newton's

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

Stabilizer	Dimension	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	$\Sigma=S_2\times S_2$		$\mathbf{L}^2+\mathbf{K}^2=1,\quad \mathbf{L}\cdot\mathbf{K}=0$

method with four linear solutions in Sec. IV A 1 used as germs to start nonlinear series in τ if $\Phi=H_{\rm NF}$ or S if $\Phi=n$.

We determine the positions $\{\mathbf{K},\mathbf{L}\}_{\rm SP}$ of the four stationary points using $H_{\rm NF}$ as Φ in Eqs. (49). This yields formal series with τ, i.e., n, as a parameter. Then, at each particular stationary point $\{\mathbf{K},\mathbf{L}\}_{\rm SP}$, we use the method in Sec. IV B 2 to find the value of n at given energy E as a solution to Eq. (47). Thus we obtain $n(S(E))_{\rm SP}$ as a formal power series in S. Results are shown in Table II.

C. Action and period

Each point of $\Sigma=S_2\times S_2$ defines an orbit of n in R (or $\mathcal{R}$) with angle ϕ_n the natural coordinate along the orbit. (n defines a dynamical symmetry operation with linear action in $\mathcal{R}_8$; see Sec. I B.) The dynamics of the system on the reduced phase space Σ is described by the Hamilton function $H_{\rm NF}$ in Eqs. (43a), (44), and (47). To find the trajectory in the initial phase space R we combine the trajectory on Σ with the n orbit motion (cf. Sec. I B 3). For a relative equilibrium [2] we obtain a periodic trajectory in R with ϕ_n the coordinate along it. (In this case the n orbit corresponds to an actual periodic orbit of the system.)

The coordinates $\{\mathbf{K},\mathbf{L}\}_{\rm SP}$ 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. The Hamilton function $H_{\rm NF}$ at this point defines a one-dimensional dynamical system with the action-angle variables (n,ϕ_n). Then it follows immediately (see, for instance, Chap. 10, Sec. 50B of Ref. [32]) that

$$n_{\rm SP}=\frac{1}{2\pi}\oint_{\rm PO}\mathbf{p}d\mathbf{q}, \tag{50}$$

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. (48c), the solution $n(E)$ of Eq. (47). 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 $(\mathbf{L},\mathbf{K})$. Periodic orbits correspond to the extrema of $n(E)$. In fact, the extremal values of the action integral (50) are already given as functions of energy in Sec. IV B 3 and Table II.

To calculate the KS space period Δ, we begin with its definition and use Eqs. (38) and (43a),

$$\frac{\Delta}{2\pi}=\left[\frac{dH_{\rm NF}}{dn}\right]^{-1}=\left[\frac{dH_{\rm NF}}{d\tau}S\frac{\omega}{2}\right]^{-1}=\frac{1}{2}\left[\frac{d}{d\tau}\left(H_{\rm NF}\,S\frac{\omega}{4}\right)\right]^{-1}=\frac{1}{2}\left[\frac{dS}{d\tau}\right]^{-1}=\frac{1}{2}\frac{d\tau}{dS}=\frac{1}{2}\frac{d}{dS}\left(n\frac{\omega}{2}S\right), \tag{51}$$

with functions $H_{\rm NF}$, $S(\tau)$, 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. For the same order of the normal-form, the period is approximated with lesser accuracy than the action.

In Fig. 1 we compare our normal-form predictions with the numerically refined ''exact'' values. 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 $\mathcal{T}_s$ 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 4–8 from the C_s-restricted normal form. (The fourth order is given in Table II; higher-order formulas are too large to be reproduced.) The series for the nonionizing G_4 orbit is alternating (cf. Table II). When S is large, this series wildly oscillates in low orders and settles only for orders higher than 4.

To see whether 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

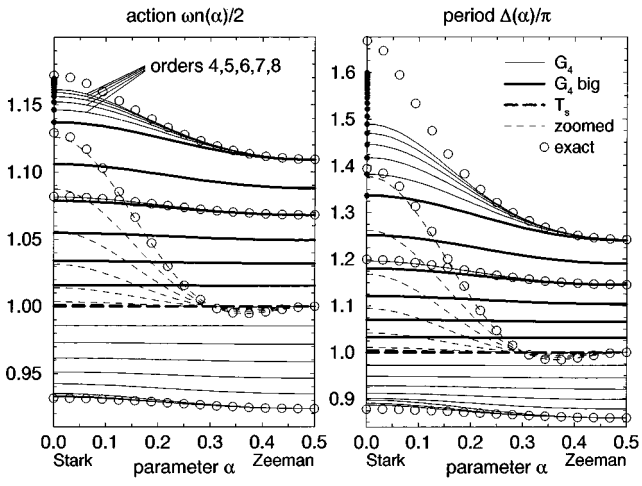

FIG. 1. Action and period of the nonlinear normal modes in the whole range between the Stark ($\alpha=0$) and Zeeman ($\alpha=\frac{1}{2}$) limit with $F_s=\cos(\alpha\pi)$, $\omega=2$ $(n\sim 1)$, and $S=0.03, 0.06, 0.09, 0.12, 0.15, 0.18$. Lines, bold for downhill (big) G_4 orbit, thin for uphill (small)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

turns into a straight line and the problem has one degree of freedom. Figure 1 demonstrates that even at order 20 the discrepancy is still significant.

D. Periodic orbits in the initial space *R*

In this section we make the correspondence between the stationary points of the normal form $H_{\rm NF}$ and the nonlinear normal modes explicit and conclude 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 formulas 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 three-dimensional (3D) Hamilton function (3).

Our first step gives an opportunity to review the geometry of the problem once again. We lifted the initial physical phase space R_6 [or C_3 with 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 $\Sigma_4=S_2\times S_2$. We also defined in Sec. II B 3 the standard coordinates $\mathcal{R}_8\to\mathcal{R}_8'$ in which the two group actions defined by n and ζ are diagonal. To define the embedding of Σ_4 into $\mathcal{R}_8$ we need local charts of Σ in terms of $(q_1',q_2',q_3',q_4',p_1',p_2',p_3',p_4')$, the coordinates on $\mathcal{R}_8'$. Each chart is a Euclidean space $\mathcal{R}_4'$. To cover the whole of $S_2\times S_2$ we use a four-chart atlas whose explicit construction is explained below.

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 to a standard construction 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 [33]. In addition to n the problem (18) has one exact integral ζ that defines the action of the 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.

To find the KS space image of a point on $S_2\times S_2$ with coordinates $(\mathbf{K},\mathbf{L})$ 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 onto 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 $p_i'^2+q_i'^2$, $i=1,\ldots,4$,

$$\phi_n=\tfrac{1}{2}(\phi_1+\phi_2+\phi_3+\phi_4), \tag{52a}$$

$$\phi_\zeta=-\phi_1-\phi_2+\phi_3+\phi_4. \tag{52b}$$

To lift Σ to $\mathcal{R}_8'$ we can fix any two phases in Eqs. (52). Thus we can fix ϕ_a and ϕ_b and obtain the chart $M^{(ab)}$ with $p_b=p_a=0$. Such a 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 (c,d) exist if $\zeta=0$ and $n\neq 0$ ($n=1$ in the scaled coordinates). Therefore, four charts with

$$(a,b)=(1,3),(2,3),(1,4),(2,4) \tag{53}$$

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

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

$\mathfrak{g}$	$2n_1$	$2n_2$	$2n_3$	$2n_4$
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. (53) 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).

The results of such calculation are shown in Figs. 2–4. Figures 2 and 3 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).

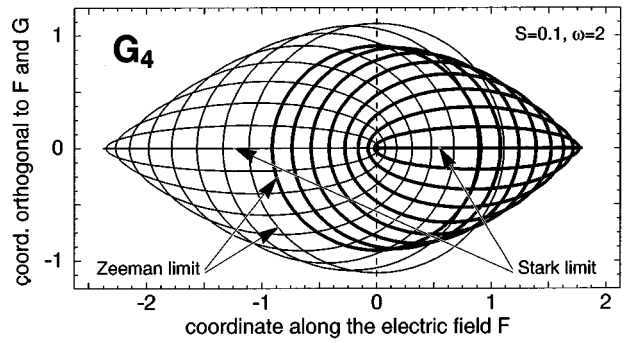

FIG. 2. Projections of the two G_4 orbits at different F_s and G_s for $S=0.1$ and $\omega=2$ $(n\sim 1)$.

Their images exhibit all symmetry properties expected in Sec. IV A 2. In particular, the G_4 orbits lie in the (e,p) plane, while the $\mathcal{T}_s$ orbits are slightly 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-field problem we analyze their stability. The geometric characteristics of stability are 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 are 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 $(++++)$ and 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

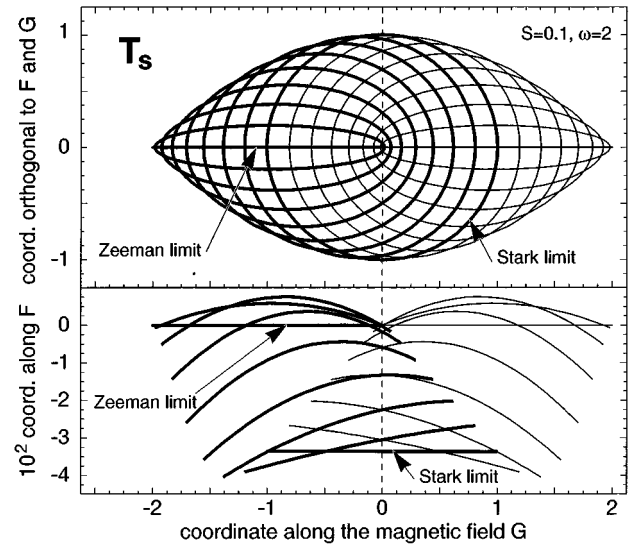

FIG. 3. Projections of the two equivalent T_s orbits at different F_s and G_s for $S=0.1$ and $\omega=2$ $(n\sim 1)$.

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 Heissian matrix in the coordinates $(J_{1x},J_{2x},J_{1y},J_{2y})$ in the linear approximation.
[c]For each G_4 mode $\omega'=\omega''$.

the larger or downhill G_4 orbit that has the maximum action. When this orbit escapes, the action becomes infinite. The two equivalent $\mathcal{T}_s$-symmetric points and 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), $i=12$, such that, for instance,

$$\cos\theta_i=2J_{ip},\quad \sin\theta_i=2\sqrt{J_{ie}^2+J_{ib}^2}, \tag{54}$$

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_{NF} in Eq. (43a) 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

$$(J_{ie},J_{ib},J_{ip})\to(J_{ix},J_{iy},J_{iz}),\quad i=1,2. \tag{55}$$

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.

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 an 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).

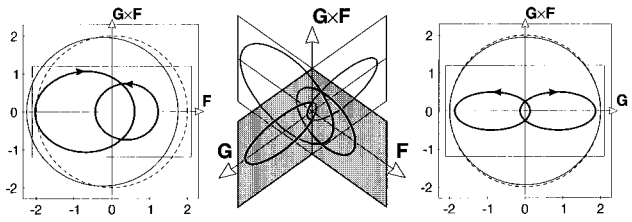

FIG. 4. Nonlinear normal modes of the crossed fields problem at $S=0.2$, $F_s=\cos(\pi/3)$, and $\omega=2$ $(n\sim 1)$. Rectangles on the left- and right-hand plots correspond to those in the center. A circle shown by broken line gives the value of the unperturbed (Coulomb) potential, the solid line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

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 $O(\tau^3)$ 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 II, so that up to $O(S^2)$ τ/S equals $1 \pm S/2$ for the G_4 orbits and 1 for the $\mathcal{T}_s$ orbits.

V. DISCUSSION

Our work presents a unified approach to the analysis of the nonlinear normal modes (NNM's); it combines explicitly the periodic-orbit study with the normal-form reduction and the methods of qualitative dynamical theory. This approach leads to the idea of tuning the crossed-field 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 parametrization. The realization of this idea is an important contribution to the crossed-field 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. The qualitative orbifold approach of Ref. [6] can be regarded as a guide to the present study and to the whole Rydberg atoms-in-field family of problems. The theory of invariants and the polynomial integrity basis (IB) construction are our major tools, indispensable both for the analysis of the normal form (the reduced Hamilton function) and for the orbifold construction. 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 study and the two complementary ways of the analysis of the NNM's define the two major directions. Expecting chaotic dynamics we can turn to the purely periodic-orbit analysis. If, however, a 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 our integrable approximation, the normal form, can be trusted and at what point the structures on the phase space associated with integrability disappear. 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

If the NNM periodic orbit is stable, the flow of the dynamical system in its vicinity has a special structure and can be reduced with regard to the total action of the small oscillations about the orbit using the method of normalization of Ref. [34]. The orbit itself lies at the center of the structure, both literally and figuratively: The structure is largely determined by such characteristics of the central orbit as stability and symmetry. Because of the latter fact such an orbit is often called an organizer [35].

In the near-equilibrium normal form of our paper the motion along all central orbits is reduced simultaneously (as the motion with coordinate ϕ_n). We can now consider each stable relative equilibrium and further normalize near it. In fact, this work begins in Sec. IV E; see also Ref. [5].

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

A reduction near each stable 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.

In the particular situation of the C_s-invariant sphere S_2 of Σ_4, we study invariant ''circles'' S_1 near the G_4 points. These circles are characterized by the position of the G_4 points in Table II and the frequency ω in Table IV. The corresponding tori in R_6 are of dimension 2 [$T_2 = S_1 \otimes S_1(\phi_n)$]. We can reconstruct these tori in R_6 or take their projection on the configuration plane (e,p) using the technique of Sec. IV D. In particular, propagating in phase ϕ_n or moving only on Σ at constant ϕ_n we can reconstruct the sections of these tori.

2. Families of periodic orbits and orbits of higher periods

When parameters G, F, and/or energy E change, stable periodic orbits can bifurcate and form genealogic families. Each family begins with the central stable orbit, a ''parent.'' At fixed G, F, and E, other periodic orbits in the family oscillate (or coil) about the central orbit with periods commensurate to the period of the latter.

For the invariant tori in the preceding subsection, our normal-form methods can predict actions and periods of the motion along their principal directions and thus select the *resonant* tori filled with periodic orbits. In reality, these tori are destroyed due to resonances that are particular to each nonlinear normal mode and cannot be taken into account by the present reduction procedure. So individual orbits that remain as a skeleton of the resonance tori cannot be predicted by our methods.

3. Chaotic dynamics and the validity of the normal form

The onset of chaotic dynamics begins with the destruction of resonant tori. If, however, the zones of irregular dynamics that emerge around the destroyed tori occupy a small phase-space volume and do not connect, 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.

B. Quantum-classical correspondence

As mentioned in Sec. II E, the normal form H_{NF} as a function of n can have immediate semiclassical (EBK) interpretation. The quantization is simple in the KS space, particularly in the diagonal representation of Sec. II B 3 where each oscillator is quantized as $n_i-\frac{1}{2}=0,1,2,\ldots$, so that $n=1,2,3,\ldots$ [use Eq. (25b)]. However, to get the quantum energy E as a function of n we should find the solution $\omega(n)$ to Eq. (43a) as a formal power series in n, so that [36]

$$-2n^2E=1+S(K_eF_s-L_bG_s)+\cdots. \tag{56}$$

This requires the n-scaled variables in Eq. (30a) and the n-scaled parametrization in Eq. (4a) rather than the energy scaling in Eq. (37) used in our Eqs. (39), (43b), and (44).

If the normal-form series works ''reasonably well,'' multiplets of quantum states with the same n, or n shells, are well separated and the H_{NF} represents an effective Hamilton operator describing the internal structure of the shells. In particular, the value of $E(n)$ defined at the stable stationary (G_4-type) points gives the splitting of the n shell. Near each G_4 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 $E(n)$ at the unstable ($\mathcal{T}_s$-type) points defines the transition region between the two systems of levels.

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

We consider $\Sigma_4=S_2\times S_2$ embedded in the Euclidean space R_6 with coordinates

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

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

1. 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. It is the natural action of G_4 on the axial (**L**) and polar (**K**) vectors. 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 that can be obtained from it by applying symmetry operations of G_4. The points in such an 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 [37]. We also call $\mathfrak{g}$ the stability, the invariance, or the local symmetry group of the orbit and of the corresponding points on $S_2\times S_2$. 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 operations $[\mathfrak{G}]$, in our case $[G_4]=4$.

If some of the components of **K** and **L** equal zero we may obtain nongeneric orbits with nontrivial 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 Eq. (A2); they form two-point G_4 orbits because for both $\mathsf{R}=T\sigma^{(eb)}$ and $\sigma^{(ep)}$,

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

Required zero components for all possible stabilizers are given in Table III. 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 onto itself by operations of $\mathfrak{g}\subset G_4$. To find a $\mathfrak{g}$-invariant manifold we consider the set of all points whose stabilizer is $\mathfrak{g}$ or greater (i.e., G_4). Results are given in Table III. For instance, to find the $\mathcal{T}_s$-invariant manifold we use Table I and consider the action of $T\sigma^{(eb)}$,

$$T\sigma^{(eb)}: s\to(K_e,K_b,-K_p;L_e,L_b,-L_p). \tag{A5}$$

It follows that the $\mathcal{T}_s$-invariant subspace is defined by four equations

$$K_p=L_p=0, \tag{A6a}$$

$$K_e^2+K_b^2+L_e^2+L_b^2=1, \tag{A6b}$$

$$K_eL_e+K_bL_b=0. \tag{A6c}$$

The geometry of this manifold is more clearly seen if we rewrite Eqs. (A6) in terms of $\mathbf{J}_1$ and $\mathbf{J}_2$ introduced in Eq. (31),

$$(J_1)_e^2+(J_1)_b^2=(L_e+K_e)^2+(L_b+K_b)^2=1,$$

$$(J_2)_e^2+(J_2)_b^2=(L_e-K_e)^2+(L_b-K_b)^2=1. \tag{A7}$$

Equations (A7) define 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

Contrary to invariant subspaces in the preceding subsection strata [15] only contain orbits with equivalent (the same) stabilizers [37]. An invariant manifold can contain several strata. Strata of nonzero dimension constitute invariant manifolds only if they are *closed*. Open strata, such as the generic stratum that is always open and dense, form invariant manifolds together with their closure. 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 that are *isolated* in their strata and such orbits are called *critical* [15]. 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 [6,7], but in the case of two orthogonal fields, no critical orbits exist and the positions of stationary points are not fixed within the strata. Restrictions on the number of stationary points on different strata and invariant manifolds follow from the Morse theory [29,30] (Sec. III C).

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[1] Our interest in the crossed-field problem as a particular application was to some extent due to the recent experimental [38] and theoretical [39,3–5,40] studies.

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[12] It should be understood that the choice of scaled field constants is not universal. Many authors tend to use the quadratic Zeeman effect as the initial point of their study. They use scaled electric-field parameters F_s of the type FG^{-2} [41] or $FG^{-4/3}$ [3], so that the Stark limit lies at $F_s\to\infty$ and this clearly implies *small* electric fields. Thus, for instance, the collapse phenomenon [7] has long remained unnoticed due to such traditional parametrization.

[13] The terms in the generator of $\mathfrak{L}$ ''replicate'' the nonresonance terms of the Hamilton function [27] 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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[24] A similar transformation is used in Refs. [42,41] [cf. their Eq. (25)] to introduce the standard representation for $\mathbf{J}_1$ and $\mathbf{J}_2$. Our choice of U agrees with direct definitions in Eqs. (14), (22), and (31).

[25] The correspondence 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) [43]. It has been widely discussed (see examples and references in Ref. [8]) and applied in the atom-in-field problems [4,44,42,41].

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