

Approximate dynamical symmetry of hydrogen atoms in circularly polarized microwave fields

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We report the discovery of an integrable three-dimensional Hamiltonian system with a velocity-dependent potential. A two-dimensional restriction of that system is (for low frequencies) a good approximation of the motion (in the polarization plane) of the hydrogen atom in circularly polarized microwave fields. An additional integral of motion of the integrable two-dimensional system (being approximate invariant for the hydrogen atom in a circular field) is used in the calculation of the classical ionization field threshold. The result is consistent with all available experimental observations.

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The physics of Rydberg atoms in a circularly polarized microwave field has drawn much attention in recent years. Ionization of Rydberg atoms in circular fields has been studied experimentally [1] and it has been observed that the ionization threshold practically coincided with the threshold in the static field. For the case of restricted motion in the plane of polarization, the ionization problem has also been treated theoretically [2]; it has been observed that classical motion is almost completely regular below the classical ionization threshold. Also, classical dynamics was used to analyze the ionization of the circular Rydberg orbits of the hydrogen atom in a circularly polarized field [3].

In this paper, we report the discovery of a completely integrable three-dimensional Hamiltonian system with velocity-dependent potential. This system is a very good approximation for bounded motions of the above realistic system for any value of intensity of microwave field, provided that the frequency is not too large. Additional integrals of motion corresponding to this system are approximate integrals for a realistic system and are responsible for the phenomena described above. To illustrate this, we have calculated (using two-dimensional restriction of our integrable system) the classical threshold field for ionization in the case of restricted motion in the polarization plane. Our results exhibit both features observed in the experiment [1]: the threshold field obeys scaling law $f_{th} \approx \text{const} \times n_0^{-4}$ (n_0 is principal quantum number of the initial state) and is practically the same as in the static-field case.

We recall that the Hamiltonian function (in atomic units) of the hydrogen atom in a circularly polarized field $H_{cir} = H_0 + f(x \cos \omega t + y \sin \omega t)$ takes, in the rotation frame [4], the following form:

$$H_{cir} = H_0 - \omega l_z + fx, \tag{1}$$

where $H_0 = p^2/2 - 1/r$, $l_z = xp_y - yp_x$, and f and ω are the amplitude and frequency of the applied microwave field. The central result of this paper is that the system defined with the Hamiltonian function

$$H = H_0 - \omega l_z + fx + \omega^2(x^2 + y^2 + 4z^2)/18 \tag{2}$$

is *integrable*, i.e., it possesses two additional integrals of motion in involution I and J , so that $\{I, H\}_{PB} = 0$, $\{J, H\}_{PB} = 0$, and $\{I, J\}_{PB} = 0$, where

$$\begin{aligned} I = & (4\omega/3)l_z[H_0 - \omega l_z + \omega^2(x^2 + y^2 + 4z^2)/18] \\ & + (8\omega^2/9)l_z^2 + f(l_y p_z - l_z p_y + x/r) + f^2(y^2 + z^2)/2 \\ & + (\omega f/3)(3xl_z - p_y r^2 + zl_x) \\ & - (\omega^2 f/9)x(x^2 + y^2 + 2z^2) \end{aligned} \tag{3a}$$

$$\begin{aligned} J = & \omega(l_x p_y - l_y p_x + z/r) + \omega^3 z(x^2 + y^2)/9 \\ & - 3fl_x/2 - (\omega f/2)xz. \end{aligned} \tag{3b}$$

We immediately see that for the restricted motion in the plane $z = 0$ [invariant for both Hamiltonian functions (1) and (2)], we have the two-dimensional integrable system with Hamiltonian function

$$H' = H_0 - \omega l_z + fx + \omega^2(x^2 + y^2)/18. \tag{2'}$$

Here the additional integral of motion is given by the restriction of the function I to the polarization plane ($z = p_z = 0$), while the second integral J vanishes (for $z = p_z = 0$). It is now natural to view the system (1) as if it has emerged from perturbation of the Hamiltonian function (2), i.e., $H_{cir} = H - \omega^2(x^2 + y^2 + 4z^2)/18$. One can expect that the perturbation is small, at least for ω not too large and for bounded motions when the electron stays in the vicinity of the nucleus. Moreover, the Hamiltonian function H' in Eq. (2'), in fact, corresponds to one realistic system: It is the hydrogen atom in the presence of both a circularly polarized laser field and a static magnetic field orthogonal to the plane of the polarization, of course with specially chosen light frequency and magnetic-field intensity.

We shall now discuss the methodology that we have used to find the above integrable Hamiltonian function (2'). It is based on the extension of the method developed by Hall [5] for the search for exact and approximate invariants of a given Hamiltonian system in the form of a polynomial in momenta, and represents an improvement of the old Whittaker method [6]. Our starting point is the two-dimensional variant of the Hamiltonian function

H_{cir} in Eq. (1), which after introducing semiparabolic coordinates $x = (u^2 - v^2)/2$, $y = uv$, and regularization, takes the form

$$\kappa = u_t^2/2 + v_t^2/2 + w \equiv 2, \quad (4)$$

where u_t and v_t are the velocities

$$\begin{aligned} u_t &= p_u + (\omega/2)v(u^2 + v^2), \\ v_t &= p_v - (\omega/2)u(u^2 + v^2), \end{aligned} \quad (4a)$$

and w is the potential

$$\begin{aligned} w &= -\alpha(\omega^2/8)(u^2 + v^2)^3 + (f/2)(u^4 - v^4) \\ &\quad - E(u^2 + v^2), \quad \alpha = 1. \end{aligned} \quad (4b)$$

E is the energy of the system. We have introduced, for future convenience, a parameter α in the potential (4b). Our task is to examine whether the Hamiltonian function (4) allows for the integral of motion, which is quadratic in momenta. Following Hall [5], we write the invariant as a polynomial quadratic in velocities

$$I = a_1(u_t^2 - v_t^2) + 2a_2u_tv_t + b_1u_t + b_2v_t + c/2,$$

where a_1 , a_2 , b_1 , b_2 , and c are unknown functions of coordinates u and v to be determined from the condition $\{I, \kappa\}_{\text{PB}} = 0$. In this way, one obtains for the unknown functions an overdetermined system of coupled partial differential equations (PDE), which allows no nonzero solution for $\alpha = 1$ in Eq. (4). It turns out that only if $\alpha = 8/9$ the system of PDE for a_1 , a_2 , b_1 , b_2 , and c can be solved and the solution is unique giving a new Hamiltonian function κ' with an additional integral of motion. It is clear that at least for the bounded motion, the new integrable system (with $\alpha = 8/9$) is very close to the old one (with $\alpha = 1$); the difference between the two Hamiltonians being the small term $(\omega^2/72)(u^2 + v^2)^3$. The resulting Hamiltonian function of the integrable system, when rewritten in Cartesian coordinates, is just that given above in Eq. (2'), and the corresponding integral of motion is given by Eq. (3a) with $z = p_z = 0$.

The generalization of the above-method function to the three-dimensional variant of the problem in Eq. (1) was much more complicated [10]. The starting point was a Hamiltonian function $H_\lambda = H_{\text{cir}} + \omega^2(x^2 + y^2 + \lambda z^2)/18$, where λ was an adjustable parameter (like α before). We then tried to find a value λ_0 for which the Hamiltonian H_{λ_0} allows two integrals of motion at most cubic in momenta. The result of that search is given in Eqs. (2), (3a), and (3b).

To illustrate how good the approximation is to the Hamiltonian function κ , Eq. (4), with $\alpha = 8/9$, to the one with $\alpha = 1$, we have compared their Poincaré surfaces of section (SOS). Figure 1(a) shows the SOS corresponding to the Hamiltonian function (4) with $\alpha = 1$, i.e., to the motion restricted in the plane of polarization of the hydrogen atom in the circularly polarized microwave field. The surface of section is defined by $u = 0$, $u_t > 0$ [note that for $u = 0$, $v_t \equiv p_v$, see Eq. (4a)]. The open line is the boundary of the classically allowed motion. Figure 1(b) depicts the SOS of the integrable Hamiltonian function

(4) with $\alpha = 8/9$, i.e., of the Hamiltonian function (2'). The parameters are chosen to correspond to the typical situation of the experiment done by Fu *et al.* [1]. E is equal to the energy of the hydrogenic level $n = 46$, the frequency is $\omega = 8.5$ GHz, and the intensity of the electric field is $f = 0.667|E|^2$, i.e., it is well above the static field at the saddle point ($= |E|^2/4$). From the first SOS [Fig. 1(a)], we see that even above the saddle-point energy, the Hamiltonian function H_{cir} , Eq. (1), supports bounded motion (in the plane of polarization). Further, the comparison with the second SOS [Fig. 1(b)] shows that for the chosen (experimental) values of parameters this bounded motion practically coincides with that of the integrable Hamiltonian H' , Eq. (2'), except in the very small region at the boundaries that separate bounded from unbounded (i.e., corresponding to ionization) motions. This small discrepancy is due to the fact that the separatrix of Fig. 1(b) consists of the stable and unstable manifolds of two unstable periodic orbits and is, therefore, most sensible to the perturbation. [Nevertheless, the separatrix from Fig. 1(b) may be considered as a good approximation to the boundary between bounded and unbounded motions in Fig. 1(a).] We emphasize that (for small enough ω) the *bounded* motion of the realistic system practically coincides with the corresponding motion of the integrable

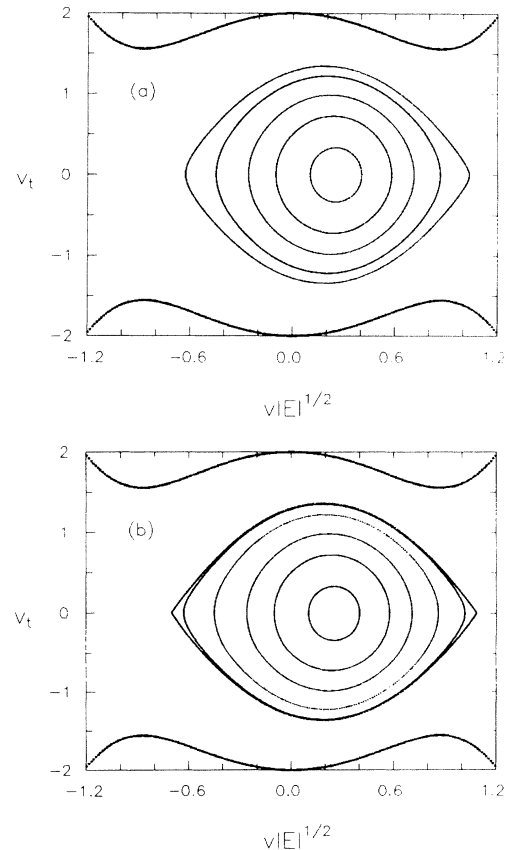


FIG. 1. Poincaré surfaces of section (in atomic units), $u = 0$, $u_t > 0$, corresponding to the Hamiltonian function (4) with (a) $\alpha = 1$, (b) $\alpha = 8/9$. $\omega = 8.5$ GHz, $E = -2.36 \times 10^{-4}$ a.u., $f = 3.72 \times 10^{-8}$ a.u.

Hamiltonian (2') for *any* field intensity f . If, e.g., one increase f , the volume of the phase space filled by bounded trajectories of the realistic system shrinks (analogously to the static-field case) and the perturbation term $\omega^2(x^2+y^2)/18$ is even smaller. (Of course, unbounded trajectories of the realistic system are not approximated at all with integrable Hamiltonian H' because for them the perturbation increases even for small ω .) Therefore, we shall use (see below) the integrable system as an approximation, to calculate ionization field thresholds of the realistic system, or the field values for which any initially bounded trajectory ionizes (breaks up). For that, it is enough that *bounded* trajectories of the realistic system are well approximated with the corresponding trajectories of the integrable system, again for small enough ω .

We further examine the range of ω for which two systems are close to each other. The empirical investigation of SOS' revealed that (for any f) (a) if frequencies are low (as in the experiment by Fu *et al.* [1]), $\omega E^{-3/2} < 0.55$, bounded motion of the realistic system coincides with the corresponding motion of the H' ; (b) for higher frequencies, $0.55 < \omega E^{-3/2} < 1$, bounded motions supported by the Hamiltonian H_{cir} are still very well described by the Hamiltonian H' but the regions of the phase space filled with corresponding motions in the two cases do not coincide; (c) for even higher frequencies, $\omega E^{-3/2} > 1$, the two systems are not close any more, moreover parts of phase space filled with chaotic motion are observed in the case of H_{cir} [7].

Now we turn our attention to the problem of ionization. In the experiments [1] on the ionization of Rydberg (Na) atoms by a circularly polarized microwave field, it is observed that the threshold field obeys the scaling law $f_{\text{th}} = 1/16n^4$, which is the same as in the static-field case and much above the threshold field in the case of the linearly polarized field $1/3n^5$. On the other hand, the threshold field for the hydrogen atom in the linearly polarized field is $1/9n^4$ [1,8]. Hence, it was expected [1] that in the case of the hydrogen atom and circular field the threshold should be above $1/9n^4$ and close to the value in the static-field case. After our work was completed, we found out that indeed, the most recent experiment [11] on the hydrogen atom confirmed such expectations and gave for the threshold law approximately $1/6n^4$, which is in excellent agreement with our results (see below).

We shall now use the Hamiltonian function H' as a zeroth-order approximation to H_{cir} , Eq. (1), and apply it to the calculation of the classical ionization field thresholds. (We emphasize that our method is an alternative to previous theoretical considerations [2,3,7,9], and that it has no connections to saddle-point analysis. We shall determine the ionization field threshold according to the experimental observation [1], i.e., the microwave field that produces 50% ionization.

We assume that the circular microwave field is adiabatically switched on, i.e., that the parameter f in the Hamiltonian function (2') is an adiabatically slow function (otherwise unspecified) of the time starting from zero, i.e., $\dot{f}(t) \ll 1$, $f(0)=0$. Therefore, since for $t=0$ the circular field is switched off, the natural choice for the initial state

of the system is the classical microcanonical ensemble of initial conditions on the energy surface (of the two-dimensional unperturbed hydrogen atom) with a given value of $E_0 = -1/2n_0^2$ (where n_0 is the total action corresponding to the principal quantum number). These initial conditions lie on certain (family of) tori in the phase space of the integrable system Eq. (2'), which is now seen as a function of parameter f , $H'(f)$, and f is slowly increased from zero. Recall that from the adiabatic theory it follows that if f changes slowly enough with time actions corresponding to given torus $I_1(f(t))$, $I_2(f(t))$ are adiabatically invariant. Using the additional integral of motion, Eq. (3a), we can trace the deformation of invariant tori of the Hamiltonian $H'(f)$ as the field intensity f is increased from zero to any given value and determine the field values for which any given torus eventually bifurcates, which corresponds to breaking up (ionization) of the corresponding torus of the realistic system Eq. (1).

One finds that of all the (bounded) trajectories in the initial ensemble, the first one to "ionize" (to become unbounded, scattering trajectories) is the circular orbit (in the nonrotating frame) of the unperturbed hydrogen atom rotating in the same direction as the field and possessing maximum value for the angular momentum $l_z = n_0$ (for $f=0$, l_z is an integral of motion). The last to ionize is the circular orbit rotating in the direction oppo-

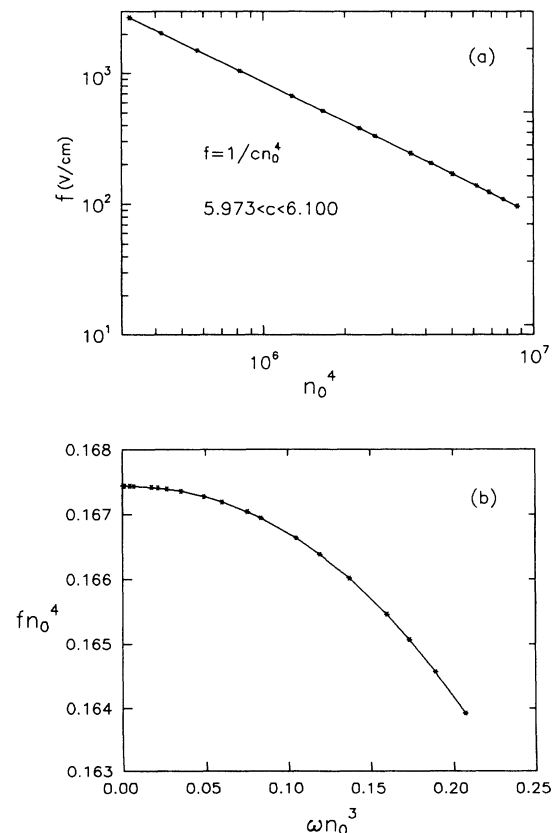


FIG. 2. (a) The ionization threshold field f as a function of the initial total action n_0 (principal quantum number) for $\omega = 8.5$ GHz. (b) Dependence of the scaled threshold field $f_{\text{th}} n_0^4$ on the scaled frequency ωn_0^3 .

site to the field ($l_z = -n_0$). Therefore, half of the initial (microcanonical) ensemble will be ionized when the field intensity reaches the value for which the trajectories initially with $l_z=0$ become unbounded. (As indicated before, the threshold in experiments [1] and [8] was defined as the microwave field producing 50% ionization.) Using the additional integral of motion, Eq. (3), we can determine the field value for which the torus (initially with $l_z=0$) breaks up. The result of such a calculation is shown in Fig. 2(a) where we give the ionization threshold fields as a function of the initial total action n_0 , for $\omega=8.5$ GHz and $n_0=24-55$. As in the experiments [1,11], the threshold practically obeys the scaling law $f_{\text{th}} \cong 1/cn_0^4$ characteristic for the (classical) static-field case. The change of the parameter c (5.973–6.100) in the scales of Fig. 2(a) is not observable. The fact that the scaling law is not quite exact is illustrated in Fig. 2(b) where we have given the dependence of the scaled threshold field $f_{\text{th}}n_0^4$ ($\cong 1/c$) on the scaled frequency ωn_0^3 . (However, note that in the same range of the scaled frequency, the change of the parameter $f_{\text{th}}n_0^4$, 0.168–0.164, is negligible compared with that of fn_{sd}^4 , 0.06–0.005, see Ref. [9], where $-1/2n_{\text{sd}}^2$ is the saddle-point energy for the given field intensity f .)

For comparison, we have also calculated the field

thresholds for the case of static field where the scaling law is exact. In the case of the two-dimensional hydrogen atom (for 50% ionization), we have obtained for the scaling constant $c_{s2}=5.972$, which is very close to the values obtained in the case of a circularly polarized field (see Fig. 2). In the three-dimensional (static-field) case, we have obtained $c_{s3}=5.783$. The small difference ($\approx 3\%$) between c_{s2} and c_{s3} clearly indicates that the two-dimensional model should also be satisfactory in the case of the microwave field.

In summary, using the discovered approximate dynamical symmetry of the hydrogen atom in a circularly polarized microwave field, we have calculated the ionization field thresholds, which are completely consistent with the previous experiment on an Na atom [1], i.e., they obey the scaling law and are very close to the threshold in the static-field case. Further, the most recent experiment [11] on the highly excited H atom has confirmed our prediction of the “exact” threshold law expression.

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