Classical dynamics and localization of resonances in the high energy region of the crossed fields hydrogen atom

Frank Schweiner, Jörg Main, Holger Cartarius, and Günter Wunner
Institut für Theoretische Physik 1, Universität Stuttgart, 70550 Stuttgart, Germany
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We follow the quasi-Penning resonances of the hydrogen atom in crossed external fields to high energies and field strengths observing structural changes and uncovering their bifurcation behavior. The appearance of a stability top and a cusp bifurcation are reported. Another orbit $B_2$ of the same structure is found in the observed parameter space becoming completely stable in a region where the classical Kepler orbits are already unstable. By quantum-mechanically exact calculations we prove the existence of signatures in quantum spectra belonging to these orbits. Husimi distributions are used to compare quantum-Poincaré sections with the extension of the classical torus structure around $B_2$. Since periodic orbit theory predicts that each classical periodic orbit contributes an oscillating term to photoabsorption spectra, we finally give an estimation for future experiments, which could verify the existence of these stable orbits $B_2$.

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I. INTRODUCTION

The hydrogen atom in crossed electric and magnetic fields is a simple example of a non-integrable physical system, which has up to now been investigated for almost one hundred years, theoretically [1–5], as well as experimentally [3–14]. Furthermore it has been used for studies on phenomena like Ericson fluctuations [8–10] or Arnold’ diffusion [6]. Even quantum dots [16] and excitons [17] in condensed matter physics can be explored using the findings attained from the hydrogen atom in crossed fields.

One of the major purposes in recent decades was to uncover how chaos, which can be observed in a classical treatment [18–20], shows itself in quantum spectra, since the Schrödinger equation is, due to its linearity, not capable of producing chaotic behavior [5, 20–26]. Nevertheless new phenomena occur in crossed fields: the so-called quasi-Penning resonances [27]. From a classical point of view these resonances describe a movement of the electron which is localized around a saddle point in the potential, the Stark saddle point. The possible appearance of wave functions localized far away from the nucleus led to a series of further investigations [27–32], since they can play an important role in the ionization process. Transition state theory predicts classical orbits localized around the Stark saddle point and states that all ionizing orbits have to pass the vicinity of this point [33–36]. Even though Clark et al. [27] already proved their existence in 1985, it was not until 2009 that first signatures of these orbits were found in calculated quantum spectra [37]. The classical stability behavior of the quasi-Penning orbits had first been investigated by Flüthmann in 1994 [38], who uncovered a stability top when following these orbits up to high energies.

It is the purpose of this paper to perform more precise calculations on the stability of these orbits and to uncover the bifurcation behavior as well as the processes taking place around the stability top. We will show that a cusp bifurcation with regard to the energy and the scaled field strength occurs in which another orbit of the same structure is involved. This orbit, becoming completely stable in a specific area of parameter space, is the starting point for semiclassical and quantum mechanical calculations, which will demonstrate that signatures of these orbits at high energies and field strengths can be found in accurately calculated quantum spectra.

In Sec. II the system is introduced, and a scaling of parameters as well as a regularization of coordinates are carried out. A comparison between exceptional points and a classical cusp bifurcation is drawn. The classical stability of the quasi-Penning resonances and their bifurcation behavior at high energies and field strengths are presented in Sec. III. An introduction in the semiclassical and exact quantum mechanical calculations performed is given in Sec. IV, before according results are discussed in Sec. V. In Sec. VI a short summary is given and conclusions are drawn.

II. CLASSICAL CALCULATIONS

A. Hamiltonian, monodromy matrix and regularized coordinates

The classical Hamiltonian of a hydrogen atom in a constant electric field $F = F\hat{e}_x$ and a constant magnetic field $B = B\hat{e}_z$ reads in Hartree units

$$H = \frac{1}{2}p_x^2 - \frac{1}{2}\frac{1}{r} + \frac{1}{2}BL_z + \frac{1}{8}B^2 (x^2 + y^2) + Fx,$$  \hspace{0.5cm} (1)

with $L_z = xp_y - yp_x$. In the following we shall take advantage of a scaling property of the Hamiltonian enabling us to deal with only two independent variables, the scaled energy and the scaled field strength

$$\tilde{E} = EB^{-2/3}, \tilde{F} = FB^{-4/3}.$$  \hspace{0.5cm} (2)
Without further usage of the tilde sign the Hamiltonian is of the same shape as in Eq. (1) when setting $B = 1$. Defining $\gamma = (r, p)^T$, we want to find periodic solutions of the Hamiltonian equations of motion

$$\frac{d}{dt} \gamma = J \frac{\partial H}{\partial \gamma}, \quad \text{with} \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{3}$$

The Stark saddle point is characterized by the fixed-point condition $\gamma = 0$, yielding its position $r_{SP} = (-1/\sqrt{F}, 0, 0)^T$ and energy $E_{SP} = -2\sqrt{F}$. The stability of orbits is investigated using the monodromy matrix $M$. $M$ describes in a linear approximation the relative behavior of two trajectories $\gamma^{(1)}$ and $\gamma^{(2)}$ in time \cite{39}.

$$\gamma^{(1)}(t) - \gamma^{(2)}(t) = M(t) \left( \gamma^{(1)}(0) - \gamma^{(2)}(0) \right). \tag{4}$$

The eigenvalues of $M(t)$ therefore indicate whether a variation of the initial conditions of a periodic orbit leads to exponential divergence or a trajectory remains in the vicinity of the periodic orbit for all times. In the case of a Hamiltonian system the energy conservation leads to two variational directions not affecting the system’s behavior. The corresponding eigenvalues hence take on the value of 1. Omitting of these directions one obtains the monodromy matrix $M$, which can be determined by its equation of motion

$$\frac{d}{dt} M = J \frac{\partial^2 H}{\partial \gamma^2} M, \quad \text{with} \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad M(0) = 1. \tag{5}$$

To prevent a divergence of the momentum $p$ near the nucleus the Kustaanheimo-Stiefel regularization of coordinates \cite{40, 41} is used,

$$r = L(U)U = \frac{1}{2} \begin{pmatrix} U_3 - U_4 & U_1 - U_2 \\ U_4 & U_3 - U_2 \\ U_1 & U_2 - U_3 - U_4 \\ U_2 - U_1 - U_4 & U_3 \end{pmatrix} U, \tag{6a}$$

$$p = \frac{1}{r} L(U)P, \tag{6b}$$

$$dt = 2r \, dr. \tag{6c}$$

The equations of motion (3) and (5) remain the same except for the replacements $\gamma \to \Gamma = (U, P)^T$ and $t \to \tau$. The Hamiltonian then reads

$$H = \frac{1}{2} p^2 - \left[ E - F (U_1 U_3 - U_2 U_4) \right] U^2 + \frac{1}{2} \left[ (U_1 P_2 - U_2 P_1) \left( U_3^2 + U_4^2 \right) \\ + (U_3 P_4 - U_4 P_3) \left( U_1^2 + U_2^2 \right) \right] \tag{7}$$

$$+ \frac{1}{8} U^2 \left( U_1^2 + U_2^2 \right) \left( U_3^2 + U_4^2 \right) + \frac{1}{2} \left[ \left( U_1 P_2 - U_2 P_1 \right) \left( U_3^2 + U_4^2 \right) \\ + \left( U_3 P_4 - U_4 P_3 \right) \left( U_1^2 + U_2^2 \right) \right] \tag{8}$$

By integrating two further equations along with the Hamiltonian equations of motion one obtains the periods and actions of the orbits:

$$\frac{d}{d\tau} t = U^2, \tag{9}$$

$$\frac{d}{d\tau} S = \frac{1}{2} \left[ (U_1 P_2 - U_2 P_1) \left( U_3^2 + U_4^2 \right) + (U_3 P_4 - U_4 P_3) \left( U_1^2 + U_2^2 \right) \right]. \tag{10}$$

The transformation (6) is not bijective. For this reason the inversion,

$$U = \begin{pmatrix} \sqrt{r + z} \cos \left( \frac{\phi + a}{2} \right) \\ \sqrt{r + z} \sin \left( \frac{\phi + a}{2} \right) \\ \sqrt{r - z} \cos \left( \frac{\phi - a}{2} \right) \\ \sqrt{r - z} \sin \left( \frac{\phi - a}{2} \right) \end{pmatrix}, \tag{10}$$

contains an additional parameter $a$, which, without loss of generality, we will set to the constant value $a = 0$.

**B. Cusp bifurcation and exceptional points**

A cusp bifurcation, appearing in systems with at least two parameters $a$ and $b$, is described by the normal form \cite{42}

$$\dot{x} = \frac{4}{27} x^3 + ax + b. \tag{11}$$

We choose the factor in front of $x^3$ as $\frac{4}{27}$ instead of 1 to simplify the results. When calculating the fixed points of Eq. (11) one finds three real solutions for $a < 0$ and $|b| < (-a)^{3/2}$. The two boundary lines of this area are tangent bifurcation lines, along which two fixed points coincide. In the remaining parameter space only one real solution can be found. A specific attribute of the cusp bifurcation shows a similarity to exceptional points: Following one fixed point around the cusp point, which is located at $(a, b) = (0, 0)$, along a circle

$$(a, b) = (-r \cos \varphi, -r \sin \varphi), \quad \text{with} \quad \varphi \in [0, 2\pi) \tag{12}$$

it can be transformed into another one. This phenomenon appears in the case of exceptional points, too. An exceptional point, firstly described by Kato \cite{43}, marks the coalescence of at least two resonances (or more precisely: eigenvalues and corresponding eigenvectors) of a complex Hamiltonian in an at least two-dimensional parameter space \cite{44, 47}. Encircling the exceptional point in parameter space the resonances permute. In the case of an EP2 two resonances interchange and the initial situation can be restored after two cycles (Fig. 1, and 4). This can be described by the normal form of a tangent bifurcation

$$\dot{x} = x^2 - \mu, \tag{13}$$
when choosing the parameter $\mu$ to be complex. The two complex fixed points can then be interchanged by encircling the exceptional point $\mu = 0$ along the unit circle in the complex plane ($\mu = e^{i\varphi}, \varphi \in [0, 2\pi]$). Similarly, the behavior of an EP$n$ can be described by the normal form

$$\dot{x} = x^n - \mu. \quad (14)$$

When encircling the exceptional point the $n$ fixed points permute and the initial situation is restored after $n$ cycles.

The cusp bifurcation shows the behavior of an EP2 and an EP3: By choosing $b = 0$ and $a = e^{i\varphi}$ one obtains an EP2-behavior. On the other hand an EP3-behavior can be obtained by setting $a$ and $b$ to $a = 0$ and $b = e^{i\varphi}$. This phenomenon was already observed in quantum mechanical calculations for dipolar Bose-Einstein condensates [46, 47]. The path of Eq. (12) with real parameters $a$ and $b$ gives rise to an ambiguity between both behaviors: If one traces two fixed points beyond a tangent bifurcation, two complex fixed points will appear. Since these two points coincide in the tangent bifurcation, it is not possible to relate one of the complex points to one of the real points, respectively. The permutation behavior cannot be determined, which is shown in Fig. 3 and 4.

III. RESULTS OF CLASSICAL CALCULATIONS AND DISCUSSION

Figure 2a shows the structure of the quasi-Penning resonances when following them up to higher energies at a fixed field strength. Since the name quasi-Penning was applied to almost elliptical orbits localized in the vicinity of the Stark saddle point and referred to the structural similarity between the equations of motion linearized around the saddle point and the stability conditions in a Penning trap we will now refer to them more generally.
FIG. 3: (Color online) Stability of $B_1$ (a) and $B_2$ (b) in dependence on the scaled energy and the scaled field strength. Along the lines marking the borders of different stability regions bifurcations take place. The stability within these regions is displayed by two upper indices. The first one refers to the stability (s) or instability (u) perpendicular to the magnetic field, the second one to the stability parallel to the magnetic field. According to the different types of stability the regions are additionally dyed by colors and grayscales. The dashed line on the left hand side in (a) marks the energy of the saddle point (SP) as a function of the field strength. Specific points in parameter space are displayed by $S_i = (F_i, E_i)$.

The differences to the case of energies slightly above $E_{SP}$ are obvious: When increasing the energy the orbit becomes more and more heart-shaped. Figure 2b shows in advance the shortest orbits in the $z = 0$-plane, which are investigated in the following.

In the following figures we indicate the stability of orbits by two upper indices added to the name of the orbit. The first one refers to the stability (s) or instability (u) perpendicular to the magnetic field. The second one indicates the stability parallel to the magnetic field. Regions of different stability are additionally dyed by colors and grayscales. The stability behavior of the orbits $B_1$ is shown in Figure 3a. After coming into existence they are at first stable parallel to the magnetic field, since the Stark saddle point is a local potential minimum in this direction. Towards higher energies they become completely unstable and may vanish in bifurcations. We note that above a specific field strength of $F_{xy,BK} = 0.481$ the right point of intersection with the $x$-axis of the orbits $B_1$ coincides with the nucleus. This coincidence takes place along the solid light blue line in Fig. 3a, which passes through the lower area of instability. Along this line the orbits $B_1$ are closed periodic orbits starting at and returning to the nucleus [71–73]. Afterwards a change in the structure takes place before the orbit vanishes in a pitchfork bifurcation with period-doubling along the right dashed line in Fig. 3a.

FIG. 4: (Color online) Stability of $B_1$ in dependence on the scaled energy and the scaled field strength. (a) is an enlargement of the rectangular area marked by dashed lines in Fig. 3a. (b) is an enlargement of the equivalently marked area in (a). The different resolutions allow for a comparison with Fig. 6 and provide a better insight in the relevant region around $F \approx 0.5, E \approx 0.6$. In the dark red area two different versions of $B_1$ exist.
In crossed fields two orbits exist, which are localized in the \( z = 0 \)-plane and which change over to the Kepler orbits \( K_1 \) and \( K_2 \). We will refer to them as \( K_1 \) and \( K_2 \). The second orbit, \( K_2 \), distinguishing itself from the first one by its sense of rotation around the nucleus, is not involved in any of the bifurcations considered and therefore not shown in Fig. 2b. The lastly mentioned dashed red line marks also a stability change perpendicular to the magnetic field of \( K_1 \), for which reason a bifurcation occurs between \( B_1 \) and \( K_1 \). Beside the bifurcation with \( K_1 \) two other bifurcations can be observed for \( B_1 \): At the stability change in \( z \)-direction pitchfork bifurcations with period-doubling occur, in which three-dimensional orbits come into being. Along the remaining line at high energies separating the white area from the area of instability a tangent bifurcation with \( B_2 \) takes place. This orbit is of the same structure as \( B_1 \), but exits only at high energies and field strengths (Fig. 3a). If one takes a closer look at the stability areas according to the \( z \)-direction one can find that they are ending in a top not only for \( B_1 \) but also for \( B_2 \). Both tops meet at the point \( S_{2,B} = (E_{2,B}, E_{2,B}) = (0.510, 0.548) \) which is located on the bifurcation line between \( B_1 \) and \( B_2 \). Therefore we conclude a continuation of the stability area of \( B_1 \) to the one of \( B_2 \).

Taking a closer look at this region of parameter space in Fig. 3b a cusp bifurcation between \( B_1 \) and \( B_2 \) is observed. Equally to the case in Sec. 1B two tangent bifurcation lines coincide in the cusp point – here \( S_{CPB} = (0.511, 0.535) \) – without continuation. Along both lines bifurcations between \( B_1 \) and \( B_2 \) occur. But while \( B_2 \) exists only in the area between both lines, \( B_1 \) exists in the complete external region and in the area between both lines twice. Starting from the continuous line we follow the orbit \( B_1 \) anticlockwise around the cusp point and again in the darker marked area until it vanishes in a tangent bifurcation along the dashed line between \( S_{CPB} \) and \( S_{xy,BK} \). Therefore two different versions of \( B_1 \), viz. \( B_{1a} \) and \( B_{1b} \) exist, which can be converted into each other by encircling \( S_{CPB} \). This behavior is the same as for the fixed points of Eq. \[ \text{Eq.} \] By allowing the coordinates and the time to become complex, the analytically continued orbits can be followed beyond the tangent bifurcations. A plot of one of the intersection points of the orbits with the \( x \)-axis vs. the angle \( \varphi \), which parameterizes the circle around \( S_{CPB} \), is shown in Fig. 5.

The left tangent bifurcation line of \( B_1 \) and \( B_2 \) in Fig. 2d leading from \( S_{CPB} \) to \( S_{xy,BK} \) coincides in \( S_{xy,BK} \) with the dashed pitchfork bifurcation line of \( B_1 \) and \( K_1 \). It continues itself towards lower field strengths as a pitchfork bifurcation line between \( B_2 \) and \( K_1 \). This line marks the upper boundary of the region in which \( B_2 \) exists. Examining the stability behavior of \( B_2 \) one can notice another interesting phenomenon: The orbit becomes completely stable in a relatively large area of parameter space (Fig. 6a). This is used as an opportunity to carry out a semiclassical quantization of these orbits and to search for signatures in exact quantum spectra in Sec. \[ \text{Sec.} \]
FIG. 7: (Color online) Stability of $D_1$ in dependence on the scaled energy and the scaled field strength. In (b) a very small region of complete stability can be observed. A cusp bifurcation takes place around the cusp point $S_{\text{CPD}}$.

Finally one last orbit localized in the $z = 0$-plane is worth mentioning. Along the dashed line in Fig. 3b describing a stability change of $B_2$ perpendicular to the magnetic field a pitchfork bifurcation with period-doubling occurs. The period-doubled orbit coming into being is named $D_1$ (compare Fig. 2). For $D_1$ both of the described phenomena can be found again! In Fig. 7b a very small region of complete stability localized at even higher energies than the stability island of $B_2$ is displayed. The cusp bifurcation takes place around the cusp point $S_{\text{CPD}}$, in which again two tangent bifurcation lines coincide without continuation. The darker marked areas denote the existence of two different versions of $D_1$: $D_{1a}$ and $D_{1b}$. We conclude that the reappearance of these phenomena indicates the possibility to find them for other orbits of even more complicated structure on and off again.

IV. SEMICLASSICAL QUANTIZATION AND EXACT QUANTUM-MECHANICAL CALCULATIONS

According to periodic orbit theory every classical periodic orbit causes a modulation in the density of states [48–57]. Oscillating modulations can also be found in photoabsorption spectra or action spectra, respectively, and are according to Gutzwiller [49] and Miller [58] located at

$$S - \sum_{i=1}^{2} \left( m_i + \frac{1}{2} \right) \varphi_i = 2\pi \left( n + \frac{\lambda}{4} \right),$$

with the action $S$, the stability angles $\varphi_i = \text{arg}(d_i)$, determined by the eigenvalues $d_i$ of the monodromy matrix, indicating the stability parallel ($\|\|$) and perpendicular ($\perp$) to the magnetic field, the Maslov index $\lambda$ and the quantum numbers $n, m_1, m_2$. These quantum numbers count the number of quanta along ($n$) and perpendicular ($m_i$) to the periodic orbit. Stable periodic orbits cause modulations of the density of states, which can be described by $\delta$-function peaks, while unstable orbits cause broadened peaks described by Lorentzians [49]. The width of these Lorentzians is given by $\sum_{i=1}^{2} |d_i|$. Since we did not calculate the Maslov index of $B_2$, we assume in the following $\lambda = 1$, which will supply the expected agreement between semiclassical and quantum-mechanical results.

The quantum-mechanical resonance spectra and wave functions are determined as described in [59]: The Schrödinger equation with the Hamiltonian (1) is rewritten in dilated semiparabolic coordinates [37, 60]

$$\mu = \frac{1}{b} \sqrt{r + z}, \quad \nu = \frac{1}{b} \sqrt{r - z}, \quad \text{and} \quad \varphi = \arctan \frac{y}{x}. \quad (16)$$

The parameter $b = |b| e^{i\vartheta/2}$ introduces a complex scaling of the coordinates $r$, which is necessary to determine resonances using the complex coordinate rotation method [61–63]. The Schrödinger equation then reads

$$\left[ \Delta_{\mu} + \Delta_{\nu} - \left( \mu^2 + \nu^2 \right) + 4b^2 + b^4 B \left( \mu^2 + \nu^2 \right) i \frac{\partial}{\partial \varphi} - \frac{1}{4} b^8 B^2 \mu^2 \nu^2 \left( \mu^2 + \nu^2 \right) - 2b^6 F \mu \nu \left( \mu^2 + \nu^2 \right) \cos \varphi \right] \psi = \left[ \Lambda \left( \mu^2 + \nu^2 \right) \right] \psi, \quad (17)$$

with the Laplacians

$$\Delta_{\rho} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2}, \quad \rho \in \{\mu, \nu\}, \quad (18)$$

and generalized complex eigenvalues $\Lambda = -(1 + 2b^4 E)$, related to the complex energies $E$ of resonances, the real
FIG. 8: (Color online) Comparison between quantum-mechanical and semiclassical results at $B = 1000$ T. The colorbar shows the quantum numbers $n$ obtained by semiclassical quantization of $B^2$. Positions where integer values of $n$ are taken on as well as semiclassical half-widths are displayed by lines. The real parts of the quantum-mechanical resonances are displayed by diamonds, the imaginary parts by error bars. Best agreements were obtained for $\lambda = 1$ and $m_{\perp} = 0$, $m_{\parallel} = 0$ in case of the first resonance series (a) and $m_{\perp} = 0$, $m_{\parallel} = 2$ in case of the second resonance series (b).

FIG. 9: (Color online) Comparison between semiclassical and quantum-mechanical results for the first resonance series at $B = 40$ T. The resonance widths are evidently smaller but still do not vanish within the stability island, which is marked by dashed lines.

$\times \sqrt{\frac{2}{\pi}} f_{n_m} (\mu) f_{n_m} (\nu) e^{i m \varphi}$, \hspace{1cm} (20)

with

$f_{n_m} (\rho) = e^{-\rho^2/2} L_{(n-|m|)/2} (\rho^2)$, \hspace{1cm} (21)

and the associated Laguerre polynomials $L_{\alpha}^k (x)$. In our numerical calculations the maximum number of states used is limited by the condition $n_\mu + n_\nu \leq 60$ due to the required computer memory. Since $\mu$ and $\nu$ are complex coordinates, all non-intrinsically complex parts must remain unconjugated in case of a complex conjugation [63, 64]. This means that $\psi_{n_\mu, n_\nu, m}^*$ is equal to $\psi_{n_\mu, n_\nu, m}$ except for the term $e^{i m \varphi}$ which is replaced with $e^{-i m \varphi}$.

The eigenstates

$\Psi_i (\mu, \nu, \varphi) = \sum_{n_\mu, n_\nu, m} c_i n_\mu, n_\nu, m n_\mu, n_\nu, m (\mu, \nu, \varphi)$, \hspace{1cm} (22)

$\Psi_i^* (\mu, \nu, \varphi) = \sum_{n_\mu, n_\nu, m} c_i n_\mu, n_\nu, m n_\mu, n_\nu, m (\mu, \nu, \varphi)$, \hspace{1cm} (23)

obtained as a result from the matrix diagonalization, are normalized according to

$\int d^3r \Psi_i^* (\mu, \nu, \varphi) \Psi_j (\mu, \nu, \varphi)$

$= \delta_{ij}$ \hspace{1cm} (24)

Owing to the limitation of the complex conjugation to the intrinsically complex parts the expression $\Psi_i^* \Psi_j$ is
FIG. 10: (Color online) Probability density $\varrho(r)$ of a resonance of the first series at $E = 1.95 \times 10^{-3} - 4.14 \times 10^{-5} i$, $F = 4.76 \times 10^{-6}$ and $B = 1.70 \times 10^{-4}$. One can observe an agreement with the course of the classical orbit (continuous line) in (a) and the restriction to the $z = 0$-plane in (b).

not a real quantity. The probability density is obtained as $\varrho = |\Psi_j^* \Psi_j| [65]$ instead. Finally Husimi distributions can be calculated, allowing a comparison between the classical torus structure existing around the periodic orbits and quantum-Poincaré sections [66]. To prevent a divergence of the momenta we use regularized coordinates for the Husimi distributions, too. We will show that the probability density of the observed resonances is mainly limited to the $z = 0$-plane. For that reason the calculations can be restricted to the $x$- and $y$- or $U_1$- and $U_2$-coordinate, respectively (cf. Eq. (6a) and (10)). By setting $z = 0$ one obtains

$$
\begin{pmatrix}
y \\
x
\end{pmatrix} = \begin{pmatrix}
U_2^2 - U_1^2 \\
2U_1U_2
\end{pmatrix},
$$

(25)

which is a bijection assuring $\alpha = 0$ as long as $U_2 \geq 0$ holds. The Husimi distribution [67,70] then reads

$$
P_H(U, P) = \left( \int d^2 \Xi |\Xi|^2 \Psi(\Xi) G(\Xi, U, P) \right),
$$

(26)

with a Gaussian of minimum uncertainty ($\Delta U \Delta P = 1/2$)

$$
G(\Xi, U, P) = \frac{1}{(\sigma^2 \pi)^{1/4}} e^{-\frac{1}{2\sigma^2}(\Xi - U)^2 - i(P + A(U))\Xi},
$$

(27)

the vector potential

$$
A = P + \frac{1}{2} B \left( U_1^2 + U_2^2 \right) \begin{pmatrix}
-U_2 \\
U_1
\end{pmatrix},
$$

(28)

and an appropriate adaptable squeezing parameter $\sigma = \sqrt{\Delta U/\Delta P}$. To determine quantum-Poincaré sections $U_1$ is set to the constant value $U_1 = 0$. The conjugate momentum $P_1$ is then calculated according to Eq. [7].

FIG. 11: (Color online) Probability density $\varrho(r)$ of a resonance of the second series at $E = 2.14 \times 10^{-3} - 5.87 \times 10^{-5} i$, $F = 4.73 \times 10^{-6}$ and $B = 1.70 \times 10^{-4}$. The differences to the classical orbit (continuous line) are significantly larger.
FIG. 12: (Color online) Probability density $|4U^2\psi^*(U)\psi(U)|$ of the resonance of Fig. 10 in regularized coordinates. Without the limitation of $U_2 \geq 0$ the probability density shows a second symmetry relative to the line $U_2 = 0$. The lower part ($U_2 \leq 0$) corresponds to $\alpha = 2\pi$ and is not included in the calculations of the quantum-Poincaré sections. The classical orbit intersects the $U_1 = 0$-line twice but with a different sign of the velocity $V_1$ in $U_1$-direction.

V. RESULTS OF QUANTUM-MECHANICAL CALCULATIONS AND DISCUSSION

Since the classical calculations have been carried out for scaled energy values and scaled field strengths one of the three parameters $E, F$ and $B$ can now be chosen arbitrarily in quantum-mechanical calculations. In the following we will set $B$ to fixed values while the other parameters are calculated according to Eq. (2) and the location of the stability island. Figure 8 shows first results at $B = 1000$ T. Two series of resonances were found, which can be traced down to lower energies. It is supposed that this retracing will end in the resonances described in [59]. The energetic distance according to the real part of the energy is almost the same within both series while the widths differ strongly between the two series. Assuming that the resonances of smaller widths (first series) represent a quantum-mechanical ground state and the other ones (second series) an excited state, semiclassical calculations are carried out to the quantum numbers $m_\perp = 0, m_\parallel = 0$ and $m_\perp = 0, m_\parallel = 2$, respectively. Since we consider only states of even parity in our quantum-mechanical calculations, the state with $m_\perp = 0, m_\parallel = 2$ must be the first excited state appearing in the spectra. As concerns the positions of the resonances a very good agreement between semiclassical and quantum-mechanical results is achieved. By contrast, differences can be found in the widths of the resonances. A good agreement is only achieved far away from the stability island. The expected decline of resonance widths within the stability island, proving the existence of quantum-mechanical bound states related to the classical stable orbits $B_2$, is not observed and will only show up at lower magnetic field strengths. When calculating Poincaré sections of the classical torus structure existing around the periodic orbit one uncovers that this structure is very small, too small to be resolved in quantum-mechanical calculations at $B = 1000$ T.

FIG. 13: (Color online) Comparison between quantum-Poincaré sections (shown by colorbar) and classical torus structure. The dashed lines display the borders of the classically permitted region. Since the Hamiltonian is a quadratic function of the momentum, there are two possibilities to choose $P_1$ when calculating the section. These both solutions differ from each other in the sign of the velocity $V_1$ in $U_1$-direction. Therefore agreements with only one part of the torus structure can be achieved at any time. The colorbar is chosen equal to compare both results. We set $\sigma$ to the constant value $\sigma = 2$.

Due to the expansion of this structure with a decreasing value of $B$ (note that $r = \tilde{r}B^{-2/3}$) one expects a
better resolution at lower field strengths. The increasing quantum number of \( n \) makes it necessary to increase the number of basis functions used in order to ensure a convergence of the quantum-mechanical calculations. Within the limitation of \( n_p + n_F \leq 60 \) it is possible to follow the resonances down to \( B = 40 \) T. Figure 9 shows that even at this field strength the resonance widths do not vanish within the stability island. The probability densities (Fig. 10 and 11) exhibit instead a partially good agreement with the course of the classical orbit. Differences can be explained by the fact that the calculated wave function is only a snapshot while the resonance itself is a time evolving and finally decaying state. It can be observed that the larger values of the probability density are taken on in the \( z = 0 \)-plane when regarding the first resonance series. In case of the second resonance series the extension in the \( z \)-direction is much larger.

The calculated quantum-Poincaré sections are compared with the classical ones in Fig. 15. As expected, the torus structure is, especially in direction of the momentum \( P_z \), much smaller than the quantum-mechanical structure.

Finally we want to estimate at which field strengths a solution of the classical structure may be possible. Since the classical orbit is localized in the \( z = 0 \)-plane we regard the extension of the torus structure around the orbit in a \( z-p_z \)-Poincaré section as its classical uncertainty. Assuming that the quantum-mechanically determined uncertainty product \( \Delta z \Delta p_z = 1.59 \) for one resonance of the first series does not change to a great extent with the value of \( B \), since it is already sufficiently close to the critical value of \( \frac{1}{2} \), we obtain a coincidence not until \( B \approx 90 \) mT! This field strength is convenient for an experimental proof of the orbits \( B_2 \) in photoabsorption spectra. As it has been described, one of the intersection points of the classical orbits with the \( x \)-axis is very close to the nucleus within the relevant region around \( F \approx 0.5, E \approx 0.6 \). An existing overlap of the corresponding resonances and the lowest states (1s or 2p) of the hydrogen atom allows therefore an experimental excitation of the hydrogen atom into these resonance states. According to closed orbit theory 77,78 and periodic orbit theory 49,57 the classical periodic orbits then become noticeable in photoabsorption spectra by oscillating terms of the form \( A \sin(2\pi SB^{-1/3} + \varphi) \), in which the amplitudes depend on the stability of the orbits as well as the process of excitation. For the purpose of an experimental proof the data of a classical orbit located in the center of the stability island is given in scaled atomic units: \( F = 0.4985, \tilde{E} = 0.75, \tilde{S} = 14.7843 \). The conversion to unscaled units at the chosen magnetic field strength is obtained by Eq. 2 and \( \tilde{S} = SB^{1/3} \).

VI. SUMMARY AND CONCLUSION

Following the quasi-Penning resonances up to high energies and field strengths we could resolve their complete bifurcation behavior. We found out that only \( K_1, B_2 \) and three-dimensional orbits are involved in the bifurcations of \( B_1 \). It was shown that several phenomena appear in the region of \( F \approx 0.5, E \approx 0.6 \) including a cusp bifurcation between \( B_1 \) and \( B_2 \) as well as the appearance of a stability island for \( B_2 \). The reappearance of these phenomena when analysing the stability and bifurcation behavior of \( D_1 \) could then be interpreted as a possibility to find them on-and-off-again for orbits of even more complicated structure. The puzzle of the \( z \)-stability region of \( B_1 \) ending in a top in parameter space could be resolved by a closer examination of the stability of \( B_2 \). The results show a coincidence of two stability tops at \( S_{z,B} \), which indicates the continuation of the stability borders limiting the areas of stability in \( z \)-direction from one of these orbits to the other one.

Semiclassical quantizations of \( B_2 \) showed agreements with resonances found in exact quantum spectra. Due to further agreements between quantum-mechanical probability densities and classical orbits as well as between quantum-Poincaré sections and classical torus structure we have to conclude that signatures of the stable orbit \( B_2 \) in exact quantum spectra have been found. Owing to limited computer memory and power it is not yet possible to reach regions of several millitesla in order to find out whether the widths of the detected resonances will disappear within the stability island or not. Nevertheless we think that an experimental proof of \( B_2 \) in photoabsorption spectra at the estimated field strengths will eventually be possible.

Finally, since the widths of the observed resonances do not vanish within the stability island of \( B_2 \) and since the stability island is very close to the bifurcation lines with \( B_{1a} \) and \( B_{1b} \), we think that the orbits \( B_2 \) cannot be treated as isolated ones in a semiclassical quantization. It would be therefore preferable to perform a uniform semiclassical quantization 74,75 of the observed cusp bifurcation.

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