Classical and quantum dynamical regimes in the bound space projected dynamics of strongly driven H Rydberg atoms

R. Blümel\textsuperscript{1}, C. Hillermeier\textsuperscript{2}, and U. Smilansky\textsuperscript{3}

\textsuperscript{1} Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA
\textsuperscript{2} Max-Planck-Institut für Quantenoptik, D-8046 Garching, Federal Republic of Germany
\textsuperscript{3} Department of Nuclear Physics, The Weizmann Institute, 76100 Rehovot, Israel

Received 6 December 1989

The bound space projected dynamics of the one dimensional model of H Rydberg atoms subjected to strong microwave radiation exhibits three dynamical regimes: (i) perturbatively localized, (ii) chaotic, (iii) external field dominated. This classification holds classically as well as quantum mechanically. The spectral properties of the bound space projected dipole operator dominating regime (iii) are studied analytically. A semiclassical analysis shows that its eigenfunctions, projected on the unperturbed basis states $|n\rangle$ of the one dimensional model, decay like $n^{-3/2}$.

PACS: 05.45.+b; 32.80.Rm

I. Introduction

It is surprising that more than sixty years after the birth of quantum mechanics, the hydrogen atom, the simplest of all atoms is still at the forefront of research. Subjected to strong electric [1, 2] and magnetic [3] fields it provides the best studied example of Quantum Chaology [4], the newly created science of quantum systems which are chaotic in the classical limit. To be specific, let us consider the hydrogen atom in a magnetic field of $B \approx 6$ T, a magnetic field strength which can be generated in the lab [3]. It has been noticed by many researchers [3, 5, 6], that the hydrogenic electron will exhibit regular motion if it is in a bound state with relatively small principal quantum number $n$. In this case, the average atomic binding field $F$ is by far stronger than the effect of the externally applied magnetic field $B$. Therefore, $B$ is a small perturbation and the atomic dynamics is approximately integrable.

A completely different situation arises if the hydrogenic electron is excited to a high lying Rydberg state [3, 5, 6]. Since $F \sim 1/n^4$, it is always possible to find a range of principal quantum numbers $n$ such that $F$ is comparable in strength with the Lorentz force acting on the electron due to the presence of the $B$ field. The resulting competition between $F$ and $B$ for determining the path of the electron will drive the electron into chaos. It is therefore a well known fact that as a function of increasing principal quantum number $n$, the H atom in an external magnetic field will perform a transition from regular to chaotic motion [3, 5, 6]. The picture outlined so far, however, cannot be complete. The question is: what happens at still higher quantum numbers $n$, where the magnetic field dominates over the atomic binding forces? In the case of the hydrogen atom the answer is tricky. Since the Coulomb potential exhibits a singularity at the origin, $B$ can never globally outweigh the electric binding force $F$ and the electron's motion stays chaotic in regimes close to the proton. On the other hand, according to Bohr's rules, the average distance of the electron from the proton scales like $\sim n^2$, so that over long portions of the electron's trajectory the $B$ field indeed dominates. As a result, the electron trajectory appears regular whenever the electron enters a region in which the $B$ field is large.

The hydrogen atom in a magnetic field is a special case of a whole class of potentially chaotic systems whose classical (quantum) dynamics is governed by
the Hamiltonian

\[ H = H_0 + \mu \cdot V \]  

(1)

where \( H_0 \) and \( V \) are integrable. Usually, \( H_0 \) stands for the Hamiltonian of an integrable microscopic system, like the hydrogen atom discussed here, and \( V \) represents the external perturbation.

For "well behaved" \( H_0 \) and \( V \) and given system energy the Hamiltonian (1) has two limits. For \( \mu = 0 \) and \( \mu \to \infty \), \( H \) is integrable. Therefore a transition from regularity to irregularity and back to regularity exists for the dynamics determined by \( H \) as a function of increasing perturbation strength \( \mu \). But as the example of the \( H \) atom in a strong magnetic field shows, an analogous transition from regularity to irregularity exists for fixed \( \mu \) as a function of system energy. This means that in order to decide if a system will be regular or irregular for a given perturbation strength \( \mu \) it is not sufficient to know the magnitude of \( \mu \). It also matters in which region of phase space the system is started out to begin with.

Another representative of class (1) systems which clearly shows the phase space dependence of regularity and irregularity for a given fixed Hamiltonian \( H \) are Mg ions confined in a Paul trap [7]. In this case the ion dynamics was studied in detail both experimentally and theoretically [8]. It was demonstrated that in analogy to the case of the \( H \) atom in a strong magnetic field, the ions can be found in three dynamical regimes: (i) crystalline and quasi periodic structures for low energy, (ii) a chaotic ion heating phase for intermediate energies and (iii) a regular regime for very high excitation energies. Order \( \to \) chaos \( \to \) order transitions between the three regimes can be induced as a function of increasing ion energy. Regime (iii) is of considerable practical importance since it accounts for the large storage times which can be achieved in a Paul trap even without the presence of a cooling laser.

In this paper we focus on yet another member of class (1) systems: the \( H \) atom driven by intense microwave fields [1, 2, 9, 10]. There is strong evidence that this system exhibits a type (iii) region [11] analogous to the one encountered for the \( H \) atom in a strong magnetic field or ions in an ion trap. On the classical level, indications for a crossover from the diffusive chaotic regime to the microwave dominated, more regular high \( n \) regime were already reported by Leopold and Percival [12]. They noticed the occurrence of "extremely highly excited states" which, located at very high energies, but still bound, were very stable against ionization (see Fig. 4 in [12]). The purpose of this paper is to provide evidence, both on the classical as well as on the quantum mechanical level, for the existence of regime (iii) and its implications for the localization behavior of the wavefunction of an \( H \) Rydberg atom in a strong microwave field. If the picture of a crossover from \( H_0 \) dominated to \( V \) dominated behavior is applicable in the case of microwave driven \( H \) Rydberg atoms, then for region (iii) we should expect that the properties of the hydrogen wavefunction are determined by the external microwave field.

The case for the existence of region (iii) is developed in the following way: in Sect. II we establish pictorially the close connection between classical phase space portraits (Poincaré sections) and snapshots of the time dependent wave function of the microwave driven \( H \) atom. The three dynamical regimes are clearly distinguishable in the classical Poincaré sections as well as in the properties of the quantum mechanical wave functions. In Sect. III we study the analytical properties of the bound space projected dipole operator which determines the behavior of the wavefunction in region (iii). In Sect. IV we discuss our results and relate them to other existing theories. We conclude with Sect. V which summarizes our results.

II. The evidence

The \( H \) atom, driven by a strong microwave field, is a simple dynamical system, which can show chaotic motion and is accessible both to classical and quantum mechanical description. As far as the calculation of ionization thresholds is concerned, the relevant dynamics of microwave driven \( H \) atoms is the bound space [9–11]. The role of the continuum is to open the ionization channel which can be used as a weak probe of the bound state dynamics. The bound space dynamics also accounts for the initial time evolution of the wave function. In this section the microwave driven \( H \) atom is investigated within the framework of a one dimensional model [13]. This model is based on the assumption that the extremal states of the hydrogen atom's Stark manifold are the first states to ionize in a linearly polarized microwave field. This assumption was recently supported quantitatively by a numerical calculation of the ionization probabilities of the different Stark states [14]. In Sect. II.1, we investigate the classical version of the one dimensional model. In Sect. II.2 we calculate a representative bound space projected wave function of the driven \( H \) atom and compare its behavior with the structure of the classical phase space portraits. The comparison reveals the existence of the three dynamical regimes in the classical as well as in the quantum mechanical picture. The three regimes are in one-to-one correspondence with each other.
II.1. The classical picture

In the one dimensional approximation and in atomic units the Hamiltonian of an H atom in a microwave field is given by [13, 15]:

\[ H = H_0 + \varepsilon x \sin(\omega t), \]  
\[ (2a) \]

\[ H_0 = \begin{cases} \frac{1}{2} p^2 - \frac{1}{x^2} & \text{for } x > 0 \\ \infty & \text{for } x \leq 0, \end{cases} \]  
\[ (2b) \]

where \( \omega \) is the microwave frequency, \( p \) is the momentum of the hydrogenic electron and \( x \) is the position. The Hamiltonian (2) is also called the “SSE” or “surface state electron” Hamiltonian [15] since it describes quite accurately the dynamics of microwave perturbed 2D sheets of electrons bound to the surface of an insulator by their image charge [16]. The classical as well as the quantum mechanical properties of the Hamiltonian \( H_0 \) defined in (2b) have been studied extensively in the literature [13, 15, 17]. In order to introduce the notation, we repeat here the major steps which lead to the solution of the \( H_0 \) dynamics. We introduce Hamilton's principal function \( W \). The differential equation for \( W \), the Hamilton-Jacobi equation for the bounded motion, is given by

\[ \frac{1}{2} \left( \frac{\partial W}{\partial x} \right)^2 - \frac{1}{x} = -|E|. \]  
\[ (3) \]

Defining \( \xi = |E| x \), we have

\[ \frac{\partial W}{\partial x} = \begin{cases} \sqrt{\frac{2}{|E|}} \left( \frac{1}{\xi} - 1 \right), & \text{for } p > 0 \\ -\sqrt{\frac{2}{|E|}} \left( \frac{1}{\xi} - 1 \right), & \text{for } p < 0. \end{cases} \]  
\[ (4) \]

This differential equation can be trivially solved to yield

\[ W = \begin{cases} \sqrt{\frac{2}{|E|}} \left( \sqrt{\frac{2}{|E|} - \xi^2} + \arcsin \sqrt{\xi} \right) + C_>, & \text{for } p > 0 \\ -\sqrt{\frac{2}{|E|}} \left( \sqrt{\frac{2}{|E|} - \xi^2} + \arcsin \sqrt{\xi} \right), & \text{for } p < 0. \end{cases} \]  
\[ (5) \]

At the outer turning point, \( x_t \), of the motion we have \( p = 0 \). Therefore, \( -|E| = -1/x_t \), and \( \xi_t = 1 \). We normalize \( W \) in such a way that \( W(x = 0) = 0 \). This implies \( C_> = 0 \). At the outer turning point, \( \xi_t = 1 \), the function \( W \) must be continuous and we get \( C_> = \pi \sqrt{\frac{2}{|E|}} \). We introduce the action variable

\[ n = \frac{1}{2\pi} \int p \, dx \]  
\[ (6) \]

which can be calculated explicitly. With \( p = \frac{\partial W}{\partial x} \):

\[ n = 2 \cdot \frac{1}{2\pi} \int \frac{\partial W}{\partial x} \, dx = \frac{1}{\pi} \left[ W(\xi = 1) - W(\xi = 0) \right] = \frac{1}{|E|}. \]  
\[ (7) \]

This yields the familiar hydrogenic expression of the energy in terms of the action: \( E = -\frac{1}{2n^2} \). From (7) it is seen that the action \( n \) is a constant of the motion, i.e., \( \frac{dn}{dt} = 0 \). Therefore, transforming to a new set of canonical variables, where \( n \) is the new generalized momentum, integrates the \( H_0 \) dynamics. This transformation is accomplished by means of the generating function \( F_2(x, n) \), a function of the old coordinate and the new momentum [18]. The generator \( F_2(x, n) \) is nothing but Hamilton's principal function \( W \) expressed as a function of \( x \) and \( n \). With \( \xi = \frac{x}{2n^2} \), we have:

\[ F_2(x, n) = \begin{cases} 2n \sqrt{\frac{2}{|E|} - \xi^2} + \arcsin \sqrt{\xi}, & \text{for } p > 0 \\ \pi - 2n \sqrt{\frac{2}{|E|} - \xi^2} + \arcsin \sqrt{\xi}, & \text{for } p < 0. \end{cases} \]  
\[ (8) \]

The conjugate variable of the action, the angle variable \( \theta \), is given by

\[ \theta = \frac{\partial F_2(x, n)}{\partial n} = 2 \cdot \begin{cases} \arcsin \sqrt{\xi - \xi^2}, & \text{for } p > 0 \\ \pi - \arcsin \sqrt{\xi + \xi^2}, & \text{for } p < 0. \end{cases} \]  
\[ (9) \]

Since \( \xi \) is positive and varies from 0 to 1 and back to 0 in one closed cycle of the motion, we parametrize \( \xi = \sin^2(\eta) \), \( 0 \leq \eta \leq \pi \). According to (9), \( \theta \) is given by \( \theta = 2\eta - \sin(2\eta) \), \( 0 \leq \eta \leq \pi \), and is a unique function of \( \eta \) for \( 0 \leq \theta \leq 2\pi \). The momentum is given by \( p = \frac{1}{\xi \cot \eta} \). In summary we have:

\[ H_0 = \frac{1}{2} p^2 - \frac{1}{x} = -\frac{1}{2n^2}, \]  
\[ (10a) \]

\[ \theta = 2\eta - \sin(2\eta), \]  
\[ (10b) \]

\[ \frac{d\theta}{d\eta} = 4 \sin^2 \eta, \]  
\[ (10c) \]

\[ x = 2n^2 \sin^2 \eta, \]  
\[ (10d) \]

\[ p = \frac{1}{n} \cot \eta. \]  
\[ (10e) \]
With the help of (10) the Hamiltonian (2) can now be expressed in terms of action angle variables

\[ H = \frac{1}{2} n^2 + 2 \varepsilon n^2 \sin^2(\eta) \sin(\omega t). \]  

(11)

The equations of motion for \( n \) and \( \theta \) are

\[ \frac{dn}{dt} = -\frac{\partial H}{\partial \theta} = -\varepsilon n^2 \cot(\eta) \sin(\omega t), \]  

(12a)

\[ \frac{d\theta}{dt} = \frac{\partial H}{\partial n} = \frac{1}{n^3} + 4 \varepsilon n \sin^2(\eta) \sin(\omega t). \]  

(12b)

The set of equations (12) is singular for \( \eta = m \cdot \pi \), \( m = 0, \pm 1, \ldots \). Consider the case \( \eta \to 0 \). Then \( n \to \infty \), i.e., the electron trajectory tries to cross the separatrix \( E = 0 = \frac{1}{2} p^2 + \frac{1}{x} \) to access the region \( E > 0 \). This energy domain corresponds to continuum states and lies outside the reach of \((n, \theta)\) space, since the very definition (6) of the action variable requires the existence of closed trajectories with \( E < 0 \). On the other hand, a temporary excursion to the \( E > 0 \) domain does not necessarily correspond to ionization since the electron, trapped in an “extremely highly excited state” [12], usually returns back to the region \( E < 0 \) in the next half cycle of the external field. This can be demonstrated by considering the energy of the electron corrected for the field energy. The resulting “compensated energy” [12] stays negative. Within \((n, \theta)\) space, a way has to be found to continue the electron trajectory across the singularity. This continuation has to preserve the unitarity of the problem, i.e., we should not lose probability from \((n, \theta)\) space. It is important to impose unitarity since we are concerned with comparing the results of the classical calculations with quantum calculations restricted to the set of bounded hydrogenic states. The natural procedure which conserves unitarity is to impose a reflection condition at the singularity, i.e., \( p \to -p \) and \( x \) is continuous. The Eqs. (12) together with the reflection condition at the separatrix define the proper classical analogue of a quantum mechanical calculation which is restricted to a basis set consisting only of the bound hydrogen wave functions.

The Eqs. (12) cannot be solved analytically. In order to obtain some insight into the behavior of their solutions, we integrate (12) numerically with suitably chosen initial conditions \( n_0 \) and \( \theta_0 \). Figure 1b shows a stroboscopic picture of the phase plane \((n, \theta)\) for about 10 different choices of \((n_0, \theta_0)\). The following three qualitatively different dynamical regimes are apparent:

i) For low \( n \)-values the dominance of the Coulomb potential results in regular motion. Whenever the frequency of the microwave field and the Kepler frequency of the unperturbed electronic motion are in resonance, the electron orbits are deformed into resonance islands. Far from resonances the KAM trajectories resemble very much the unperturbed motion [15] with \( n = \text{const} \) and \( \theta = \text{const} \).

ii) For increasing action values \( n \), the Coulomb force and the microwave field become comparable in strength. The growing width of the resonance islands finally results in an overlap [19] which destroys the confining KAM trajectories between them. We see chaotic motion.

iii) Orbits in the high-\( n \)-region see the dipole interaction as the prevailing term. This is reflected in seemingly regular orbits of U-shaped structure [20], which are characterized by \( x \) being an approximate constant of the motion in the stroboscopic picture. For comparison, the right most curve in Fig. 1b shows a plot of \( x = \text{const} \) in terms of \((n, \theta)\).

This division of phase space into three qualitatively different zones is intuitively understood on the basis of the Hamiltonian (11) which consists of
two competing terms with strongly different \( n \) dependence. For low \( n \), \( H \approx H_0 = -\frac{1}{2n^2} \). Free motion dominates resulting in regular structures for \( n < 10 \). For \( 11 < n < 20 \), \( H_0 \) and \( V = 2\pi n^2 \sin^2(\theta) \sin(w_0 t) \) (and the forces derived from them) are comparable in strength, resulting in chaotic motion. The \( n^2 \) dependence of \( V \) finally wins out over the \( n^2 \) dependence of \( H_0 \) and again the phase space portrait appears regular. The U-shaped structures, however, are not to be confused with invariant curves. As mentioned in the introduction, \( H_0 \) exhibits a singularity at \( x = 0 \), resulting in chaotic motion for small \( x \). For large \( n \), however, the chaotic region will be confined to narrow strips at \( \theta \approx 0, 2\pi \) [21]. The position \( x \) of the electron changes slowly on the time scale of unperturbed motion and so do the U's which represent \( x = \text{const} \) curves. In the long run, reflecting the existence of the chaotic strips at \( \theta \approx 0, 2\pi \), the U's will form fuzzy belts until they finally dive down into the chaotic strip from where the electron can once more be ejected into the high \( n \) region (iii).

In the next subsection we calculate the quantum wavefunction of an electron started in the \( n = 10 \) island of Fig. 1b and compare its structure with the typical zone-structure of classical phase space.

11.2. The quantum mechanical picture

The Hamiltonian (2), interpreted as a quantum mechanical operator, possesses a discrete and a continuous spectrum

\[
H_0|n\rangle = -\frac{1}{2n^2}|n\rangle, \quad H_0|k\rangle = \frac{i}{2} k^2 |k\rangle
\]

with \( n = 1, 2, \ldots \) and \( k > 0 \). The states \(|n\rangle\) and \(|k\rangle\) are given by [10, 21]

\[
\langle x | n \rangle = 2n^{-5/2} x F_1(\frac{2-x}{n}) e^{-xi},
\]

\[
\langle x | k \rangle = \frac{2k^2}{(1-e^{-2i\pi k})} x F_1(1+i \cdot \frac{1}{k} \cdot 2; 2ikx).
\]

Disregarding the continuum, the full time dependent wavefunction of the hydrogenic electron governed by the Hamiltonian (2a) is given by

\[
|\psi_n(t)\rangle = \sum_{n=1}^{\infty} a_n(t)|n\rangle.
\]

The subscript \( n_0 \) labels the initial condition, i.e., \( |\psi_{n_0}(t=0)\rangle = |n_0\rangle \). The amplitudes \( a_n(t) \) satisfy the equations:

\[
i\dot{a}_n(t) = -\frac{1}{2n^2} a_n(t) \pm \sin(\omega t) \sum_{m=1}^{\infty} \langle n|\xi|m\rangle \alpha_m(t),
\]

which are derived in the usual way by inserting the ansatz (16) into the time dependent Schrödinger equation with the Hamiltonian (2a). The matrix elements \( \langle n|\xi|m\rangle \) are known explicitly. The diagonal matrix elements are given by \( \langle n|\xi|n\rangle = \frac{1}{2} n^2 \). Using (14) and the recurrence relations for Laguerre polynomials ([22], 8.976), the off diagonal matrix elements are calculated according to:

\[
\langle n|\xi|m\rangle = \frac{1}{\sqrt{n m}} \int_0^{\infty} dy e^{-\frac{1}{2}(\frac{n}{y} + \frac{1}{m})} y \left\{ \text{L}_p^{(1)}(y) \frac{\text{L}_q^{(1)}(y)}{p} \right\} 
\]

\[
-2 \text{L}_{m-1}^{(1)}(y) \frac{\text{L}_q^{(1)}(y)}{m} - 2 \text{L}_{m-1}^{(1)}(y) \frac{\text{L}_q^{(1)}(y)}{m}.
\]

Introducing the integrals ([21], Appendix 1)

\[
\text{I}_{pq}^{(n,m)} = \frac{1}{\sqrt{n m}} \int_0^{\infty} dy e^{-\frac{1}{2}(\frac{n}{y} + \frac{1}{m})} y \text{L}_p^{(1)}(y) \frac{\text{L}_q^{(1)}(y)}{m}
\]

\[
= 4^n \frac{p+1}{(m n)!} \frac{(\frac{1}{m} - \frac{1}{n})^{p+q}}{(\frac{1}{m} + \frac{1}{n})^{p+q+2}} P_{p-q-2}^{n+1} \left( \frac{n}{2m} \right) \left( \frac{m}{2n} \right).
\]

where \( P_{p,q}^{n}(x) \) is a Jacobi polynomial ([22], 8.960), the final result for the off diagonal matrix elements is:

\[
\langle n|\xi|m\rangle = \frac{1}{\sqrt{n m}} \left\{ I_{pq}^{(n,m)} - 2 I_{k+n-1, m-1, m-2}^{(n,m)} 
\]

\[
- 2 I_{k+n-1, m-1, m-2}^{(n,m)} - 2 I_{k+n-1, m-1, m-2}^{(n,m)} - 2 I_{k+n-1, m-1, m-2}^{(n,m)} - 2 I_{k+n-1, m-1, m-2}^{(n,m)}.
\]

In all our calculations we used the exact matrix elements (20) for \( n, m \leq 100 \) as well as \( n \leq 10 \) or \( m \leq 10 \). All the other off diagonal matrix elements were calculated by means of the approximate formula ([10], Appendix B):

\[
\langle n|\xi|m\rangle \approx C \cdot (1 + \delta_{n,m}) \frac{E_n E_m}{{E_n}^{3/4} + {E_m}^{1/4}} 
\]

\[
\{-1 + D \frac{E_n + E_m}{|E_n - E_m|^{1/3}} \}.
\]
where $E_n = -\frac{1}{2n^2}$, $C = \frac{2}{\pi} 6^{1/3} I(2/3) \approx 1.162$ and $D = 0.21773$. The matrix elements (21) are constructed according to [23], paragraph 51. The relative error of (21) compared with the exact matrix elements (20) is uniformly less than 4.2 $\times$ 10$^{-3}$ for all $n$, $m$, and less than 10$^{-4}$ for $n$, $m \geq 6$. The correction parameters $\epsilon_j$ can be found in [10], Table 2, for $1 \leq j \leq 10$.

For $\epsilon = 6 \times 10^{-6}$, $\omega = 10^{-3/3}$ and $n_0 = 10$, we integrated the equations of motion (17) for the amplitudes $a_n(t)$ over several hundred cycles. After every cycle, i.e., for $t = N \cdot \frac{N \cdot 2\pi}{\omega}$, where the external field vanishes, we plotted the probabilities $P(n) = |\langle n | \psi_{n_0}(t) \rangle|^2 = |a_n(t)|^2$ as a function of $n$. For more than $N \approx 10$ cycles, all probability snapshots look qualitatively the same and appear to be "frozen" in time in accordance with the widely accepted notion of a suppression of classical chaos by destructive quantum interference [9, 21, 24–26]. The interference effects result in a "localization" or "freezing" of wave packets after some initial start-up time. In Fig. 1a we plot the occupation probabilities averaged over the first 100 cycles.

Figure 1a, just like the classical picture (Fig. 1b) again shows three dynamical regimes:

(i) A strong peak at $n = 10$, representing an electron trapped in the regular island around $n \approx 10$.

(ii) Irregular fluctuations of the wavefunction in the $n$-region corresponding to the region of competitive Hamiltonians and classically chaotic motion.

(iii) A smooth powerlaw behavior in the large $n$ regime with $|\langle n | \psi_{n_0} \rangle|^2 \approx n^{-5.6}$ which corresponds to the more regular, field dominated behavior in classical region (iii).

More evidence for the existence of regime (iii) can be gathered by constructing the propagator $\hat{U}$ which propagates the one dimensional hydrogen atom over one period of the external microwave field:

$$\hat{U}|\psi_{n_0}(NT)\rangle = |\psi_{n_0}((N+1)T)\rangle.$$  

(22)

With the help of $\hat{U}$ the wave function $|\psi_{n_0}(NT)\rangle$ after $N$ cycles of the microwave field is easily computed

$$|\psi_{n_0}(NT)\rangle = \hat{U}^N |\psi_{n_0}(0)\rangle = \hat{U}^N |n_0\rangle.$$  

(23)

The propagator $\hat{U}$ contains valuable information about the time evolution of the system. Insight into the localization properties of the one dimensional hydrogen wave functions is obtained by studying the spectrum and the structure of the eigenstates of $\hat{U}$:

$$\hat{U}|\alpha\rangle = e^{i\chi_\alpha} |\alpha\rangle.$$  

(24)

The states $|\alpha\rangle$ are called the quasi energy states and the angles $\chi_\alpha$ are the quasi energies [27]. For $\epsilon = 6 \times 10^{-6}$, $\omega = 10^{-3/3}$ and a basis of 300 unperturbed $|n\rangle$ states, we constructed the propagator $\hat{U}$ and diagonalized it. Figure 2a and b show the three types of quasi energy states which were obtained.

- States strongly peaked on unperturbed $|n\rangle$ states.
- The state on the left hand side in Fig. 2a, peaked on $n = 4$, is a representative of this class of states. States of this type are found in dynamical region (i).
- Since in this region the microwave field is a small perturbation we call the strongly peaked low $n$ states "perturbatively localized".

- States, like the one shown in Fig. 2b, which appear irregular in the range $11 < n < 30$ and then decay like a power in $n$ which is close to $\sim 5$. These states correspond to the dynamical region (ii).

- States which strongly overlap with region (iii). They all have a characteristic shape which includes a ridge, an oscillatory regime and a power decay for large $n$. The power, again, is close to $\sim 5$. The right hand state plotted in Fig. 2a is a typical representative of this class of quasi energy states. Because of the powerlaw decrease of the quasi energy states in regions (ii) and (iii), we call them "powerlaw localized".

The results presented above demonstrate that the structures of the classical phase portraits are one-to-one reflected in the properties of the corresponding quantum mechanical wavefuctions. Since regime (i) and (ii) are already discussed by many authors [9, 10, 28, 29], we concentrate in the following section on regime (iii). In particular, we explain the origin of the typical structure of quasi energy states in regime (iii) and present a semiclassical theory which explains satisfactorily the powerlaw decrease of the quantum wavefunctions in regime (iii). A more detailed discussion of the above mentioned localization properties of the quasi energy states is given in Sect. IV.

We conclude this section with a curiosity. It can happen that two quasi energies are nearly degenerate. This is called a quasi energy avoided crossing [30]. In solid state physics such crossings are responsible for conductance fluctuations in mesoscopic systems [31–33]. The quasi energy states at such a crossing resemble each other in structure, since they are essentially even and odd combinations of the (isolated) crossing states before and after the actual crossing takes place as a function of system parameters. Figure 2c shows the quasi energy states of the propagator $\hat{U}$ for quasi energies $\chi_\alpha = 3.8858$ (full line) and $\chi_\alpha = 3.8883$ (dashed line). They indeed resemble each other closely and consist of a linear combination of a type (i) and a type (iii) state. Since both quasi energy states in Fig. 2c effectively connect $n = 7$ with
a whole range of high lying states, probability concentrated at $n=7$ at time $t=0$ is very efficiently transported to this range of high lying states under the action of $\hat{\mathcal{U}}$. Curiously enough, this probability transport happens without the participation of the intermediate $n$ states. Probability "worm holes" of this type are currently discussed as possible candidates for fast switches in future computer technologies \cite{34}.

Even the crossing states in Fig. 2c display the peculiar ridge and powerlaw structure. We argue that this structure is produced by the dominance of the microwave field in this regime of $n$ values. Since we treated the microwave field in dipole approximation (see (2a)), regime (iii) must reflect the properties of the dipole operator, which in our model is nothing but the bound space projected position operator. The detailed investigation of this operator will be the subject of the following section.

III. The $x$-regime

In this section we focus on the behavior of the hydrogen wavefunctions in regime (iii), i.e., in the large $n$ domain. Since in this $n$-region the microwave field dominates over the unperturbed motion represented by $H_0$, it is necessary to understand the spectral properties of the bound space projected $x$-operator. We define the bound space projector by

$$\hat{\Pi}_B = \sum_{n=0}^{\infty} |n\rangle \langle n|$$

and the bound space projected dipole operator by

$$\hat{x}_B = \hat{\Pi}_B \hat{x} \hat{\Pi}_B.$$  

We are interested in the eigenvalues $\xi_n$ and eigenfunctions $|\psi_n\rangle$ of $\hat{x}_B$

$$\hat{x}_B |\psi_n\rangle = \xi_n |\psi_n\rangle.$$  

Fig. 2a–c. Some typical quasi energy states obtained from a diagonalization of the one cycle propagator $\hat{\mathcal{U}}$ (see (22)) in a basis of 300 unperturbed $|n\rangle$ states. a Left hand side: quasi energy state corresponding to region (i) and peaked at $n=4$. Right hand side: quasi energy state corresponding to region (iii) and exhibiting the typical structure of $x_n$ eigenstates. For comparison the $x_{46}$ eigenstate $|\psi_{46}\rangle$ is also shown (dashed line). b "Irregular" quasi energy state in the classically chaotic region. c Level crossing of quasi energy states. Full line: $x_n = 3.8858$, dashed line: $x_n = 3.8883$.
It is not very difficult to diagonalize $\hat{x}_B$ in a large basis of $\hat{H}_o$ eigenstates $|n\rangle$. Thus, as a first approach, we diagonalized $\hat{x}_B$ in a space of 1800 unperturbed $|n\rangle$-states, which were chosen as the first 1800 bound $\hat{H}_o$ eigenstates (14). This way we get a first impression about the $\hat{x}_B$-spectrum and the shape of the $\hat{x}_B$ eigenfunctions. Table 1 shows the first ten eigenvalues of $\hat{x}_B$. They are discrete and behave like $\xi_n \sim n^2$. The coefficients $|\langle n|\psi\rangle|^2$ resulting from a projection of the $\hat{x}_B$ eigenstates $|\psi\rangle$ on the unperturbed states $|n\rangle$ all behave the same as a function of $n$. For small $n$ they rise like a powerlaw, exhibit a sharp threshold at some $n_1^{(o)}$, oscillate between $n_1^{(o)}$ and $n_2^{(o)}$ and then decay like a powerlaw, which can be estimated graphically to be the same for all $v$ and roughly given by $|\langle n|\psi\rangle|^2 \approx n^{-5.0}$ for $n > n_2^{(o)}$. Figure 3a (full line) shows the fifteenth $\hat{x}_B$ eigenstate as a typical representative of the whole class of $\hat{x}_B$ eigenstates. The sharp drop in the $\hat{x}_B$ eigenstates at $n = n_1^{(o)}$ is very important for the asymptotic behavior of the hydrogen atom's wavefunction. This can be seen in the following way: Assume that the hydrogen wavefunction is localized in some $n$-regime, $\bar{n}_1 < n < \bar{n}_2$, i.e.,

$$\psi_{n_0}(t) = \sum_{n = \bar{n}_1}^{\bar{n}_2} a_n(t) |n\rangle. \quad (28)$$

Since $\hat{x}_B$ is a hermitian operator in the space $\{|n\rangle\}_{n=1}^{\infty}$ of bounded $H_o$ states (14), the wavefunction (28) can alternatively be expanded in $\hat{x}_B$-eigenstates. Defining $|\psi\rangle$ as the $\hat{x}_B$-eigenstate for which $\psi_1^{(o)} = \bar{n}_2$, we have $|\langle v|\psi_{n_0}(t)\rangle| < 0$ for all $v > \bar{v}$ because of the triangular shape of the $|\psi\rangle$ states. Therefore:

$$\psi_{n_0}(t) = \sum_{v=1}^{\bar{v}} a_v(t) |v\rangle. \quad (29)$$

Table 1. The first ten eigenvalues of the bound space projected dipole operator $\hat{x}_B$. First column: exact eigenvalues obtained from a diagonalization of the $\hat{x}_B$ matrix in a space of 1800 states. Second column: semiclassical eigenvalues obtained from the zeros of (45). Third column: approximations to the semiclassical values in column 2 obtained from the zeros of (46).

<table>
<thead>
<tr>
<th>$v$</th>
<th>$\xi$, exact</th>
<th>$\xi$, semi class.</th>
<th>$\xi$, appr. s.el.</th>
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<tr>
<td>1</td>
<td>1.39214</td>
<td>1.51954</td>
<td>1.82354</td>
</tr>
<tr>
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<td>35.1382</td>
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<td>45.6010</td>
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</tr>
<tr>
<td>10</td>
<td>125.381</td>
<td>126.414</td>
<td>134.355</td>
</tr>
</tbody>
</table>

Fig. 3a, b. The state $|\psi = 15\rangle$ in various approximations. a full line: exact calculation in a basis of 2500 unperturbed $|n\rangle$ states. Dashed line: exact diagonalization simulating an infinite basis size using the DOPE scheme. b Full line: see a. Dashed line: semiclassical state $|\psi = 15\rangle$.

with

$$a_v(t) = \sum_{n = \bar{n}_1}^{\bar{n}_2} a_n(t) |\langle v|n\rangle| \quad (30)$$

Since the sums in (29) and (30) are finite, the asymptotic behavior of $|\psi_{n_0}(t)\rangle$ will be determined by the asymptotic behavior of the states $|\psi\rangle$. Since all these states show the same powerlaw behavior, i.e., $|\langle n|\psi\rangle|^2 \approx n^{-5.0}$ for large $n$ and independent of $v$, so will the wavefunction (29). Thus, the powerlaw behavior of the wavefunction shown in Fig. 1a reflects nothing but the asymptotic behavior of the $\hat{x}_B$-eigenstates.
So far, the exponent of the powerlaw was obtained graphically from a diagonalization of the $\hat{x}_p$-operator in a large but finite basis. Two questions arise immediately, which will be addressed one by one in the remainder of this section. a) Since the $\hat{x}$-matrix elements $\langle n|\hat{x}|m \rangle$ behave like $n^2$ for fixed $|n-m|$, basis truncation effects might be severe and the powerlaw might depend on the size of the basis. b) Is there an analytical way to calculate the powerlaw together with $n_1^{(\gamma)}$ and $n_2^{(\gamma)}$? To answer question a) and to rule out that we are fooling ourselves with claims which depend on the basis size, we devised a numerical scheme, which can take into account a vast amount of information of the $\hat{x}_p$-operator which lies beyond the reach of a restricted basis. The method is based on an expansion of the truncated part of the wave function in a set of discrete orthonormal polynomials (DOPO = discrete orthogonal polynomial expansion) and described in detail in [10], Appendix D. In its simplest form, one makes an ansatz for the asymptotic behavior of the $|\gamma\rangle$ eigenstates

$$
\xi^{(n)} = \langle n|\gamma\rangle = \frac{\gamma}{n^2}, \quad \text{for } n > N_B
$$

where $N_B$ is the size of the basis, $s$ is part of the ansatz and $\gamma$ is to be computed by diagonalization. The symmetric eigenvalue problem to be solved in order to determine $\xi^{(n)}$ together with $\gamma$ is

$$
\sum_{m=1}^{N_n} (m-n) \xi^{(m)} + D_n \xi^{(n)} = \xi^{(m)} \xi^{(n)}, \quad n \leq N_B,
$$

$$
\sum_{m=1}^{N_n} D_m \xi^{(m)} + F n \xi^{(n)} = \xi^{(m)} \xi^{(n)}
$$

where

$$
D_n = \beta \sum_{m>N_B} \langle m|\hat{x}|n \rangle \frac{1}{m^2},
$$

$$
F = \beta^2 \sum_{m>N_B} \frac{1}{n^2} \langle m|\hat{x}|n \rangle \frac{1}{m^2},
$$

and

$$
\beta = \left[ \sum_{m>N_B} \frac{1}{m^2} \right]^{-\frac{1}{2}}.
$$

The infinite sums in (32e)-(32f) were performed by exact summation for $n, m < 10000$ and the remainder estimated with the help of asymptotic expansions of the matrix elements (21) and conversion of the infinite sums to integrals. According to (32a, b) the vector $\xi^{(n)} = (\xi^{(n)}_1, \ldots, \xi^{(n)}_{N_B}, \xi^{(n)})$ is an eigenvector of the enlarged diagonalization problem with $x_{N_B+1, n} = x_{N_B+1, n}$ and $x_{N_B+1, N_B+1} = F$.

As a typical result, Fig. 3a shows the effect of basis truncation: The fifteenth eigenvector obtained by standard diagonalization of $\hat{x}_p$ in a basis of 2500 states is contrasted here with the result of a $s = 7/3$ DOPE calculation. The example shows that basis truncation effects are indeed severe for $n > 1000$ but do not affect neither the location of the ridge structure at $n_{max}^{(\gamma)}$, nor the point of onset of smooth behavior $n_{max}^{(\gamma)}$, nor the powerlaw decay if the bending down of an $\hat{x}_p$-eigenstate toward the end of the basis is ignored.

Beyond the estimation of basis truncation effects the presented scheme also provides more precise information about the asymptotic power $s$. The numerically calculated vector $\xi^{(n)}$ has to be consistent with the asymptotic ansatz (31):

$$
\Delta^{(n)}_{\gamma} \equiv \xi^{(n)}_{\gamma} - \frac{\gamma(s)}{(n_B)^s} \approx 0.
$$

The difference $\Delta^{(n)}_{\gamma} \equiv \xi^{(n)}_{\gamma} - \frac{\gamma(s)}{(n_B)^s}$ calculated for the parameter values $N_B = 800$ and $s = 15$ as a function of $s$ resulted in a smooth curve which cuts the $s$ axis at $s_0 = 2.27$. This value differs by less than 3% from the analytical code $s = 7/3$ (see (57)) whose derivation will be the subject of the rest of the section.

As an attempt to answer part b) of the two questions raised above, we will now show how the spectrum and shape of the $\hat{H}_0$-operator can be calculated semiclassically. In order to calculate the semiclassical expressions of the $x$ representation of the $H_0$-eigenfunctions, $\langle x|\gamma\rangle$, we need the classical generator $F(x, n)$ (see (8)) of the canonical transformation from $(x, p)$ to $(\theta, n)$ variables. According to [35], formula (2.50b), the eigenfunctions of $H_0$ in $x$ representation are given by:

$$
\langle x|\gamma\rangle = \int_{\mathbb{R}} \frac{d^2 F_2(x, n)}{\partial x \partial n} \left( \frac{1}{2\pi i} \right)^{1/2} \exp(i F_2(x, n))
$$

$$
= \sqrt{\frac{2}{\pi \eta}} \sqrt{\tan \eta} \cos \left[ n(2\eta + \sin 2\eta) - \frac{3\pi}{4} \right]
$$

where the sum in (34) is over the two possible values for the momentum $p$ for given $x$ and $n$. Here and in the following the angle $\eta$ shall be considered as a function of $\theta$ which is given implicitly in (10b). The wavefunctions (34) can be transformed into angle representation $\langle \theta|\gamma\rangle = \int \langle \theta|x\rangle \langle x|\gamma\rangle \, dx$. This requires knowledge of the semiclassical transformation ampli-
tudes \langle x | \theta \rangle \) which can be calculated according to \([35]\), formula (2.50a). Care has to be taken in the derivation of (2.50a) for a half space. In this case, e.g., \(\langle x | p \rangle = \frac{1}{2 \sqrt{\pi i}} \cos(xp), x, p > 0\) and therefore

\[
\langle x | \theta \rangle = \sum_{\pm \phi, \eta} \left[ -\frac{\partial^2 F_1(x, \theta)}{\partial x \partial \theta} \frac{1}{2 \pi i} \right]^{1/2} \exp[iF_1(x, \theta)]
\]

\[
= \sqrt{\frac{1}{\pi i (8x)}} \frac{1}{\sqrt{\sin \eta}} \cos[\sqrt{8x \cos \eta}];
\]

\(x > 0, 0 < \theta < \pi.\)

With these transformation amplitudes we get for the \(\theta\) representation of the semiclassical energy eigenfunctions (34):

\[
\langle \theta | n \rangle = \sqrt{\frac{2}{\pi}} \cos(n \theta).
\]

Introducing the action operator \(\hat{\eta} = -i \frac{d}{d \theta}\), the functions (36) are seen to be the exact eigenfunctions of \(H_0 = -\frac{1}{2} \hat{\eta}^2\) in action angle space.

We define the semiclassical operator \(\hat{x}_\theta\) as the operator analog of the classical function (10d) by replacing the action and angle \(e\)-numbers in (10d) by the corresponding quantum operators:

\[
\hat{x}_\theta = 2 \hbar \sin^2(\eta) \hat{\eta}.
\]

We are aware of the fact that other hermitian operator orderings are also possible. We shall show below that the ordering chosen in (37) provides accurate expressions for both the matrix elements of \(\hat{x}_\theta\) and its eigenvalues and shall sketch a comparison with another possible ordering.

The matrix elements of (37) in the space of the functions (36) are easily calculated. Using the integral

\[
\int_0^\pi d\eta \cos(N \theta) \sin^2(\eta) = \frac{\pi}{8 |N|} J''_{|N|}(|N|),
\]

\(N = \pm 1, \pm 2, \ldots\), we obtain:

\[
\langle n | \hat{x}_\theta | m \rangle = \frac{4nm}{\pi} \int_0^\pi d\theta \sin(n \theta) \sin^2 \eta \sin(m \theta)
\]

\[
= \begin{cases} 
\frac{1}{2} n^2 + \frac{1}{2} n J_{n}^2(2n), & \text{for } n = m \n
\frac{n m}{|n-m|} J_{|n-m|}^2(|n-m|) + \frac{n m}{n+m} J_{n+m}^2(n+m), & \text{for } n \neq m
\end{cases}
\]

According to \([23]\), paragraph 48, the semiclassical \(x\) matrix elements are the Fourier amplitudes

\[
\chi_{n-m} = \frac{1}{2 \pi} \int_0^{2 \pi} \exp(i(n-m)\theta) x(\theta) d\theta
\]

\[
= \begin{cases} 
\frac{1}{2} n^2 & \text{for } n = m \\
\frac{n m}{|n-m|} J_{|n-m|}^2(|n-m|) & \text{for } n \neq m
\end{cases}
\]

of the corresponding classical variable \(x(\theta)\). The result (39) can be found in \([36]\), formula (70, 7). Indeed, the Fourier transform (39) of \(x(\theta)\) resembles closely the result (38). We checked that (38) is a much better approximation of the matrix elements of the semiclassical dipole operator than (39) for \(|n-m| \gg 1\). For \(n \approx m\) (39) is a better approximation to the exact dipole matrix elements than (38). The difference between (38) and (39), however, is seen to vanish in the limit \(n \to \infty\).

Another apparently natural choice of hermitian operator ordering for \(\hat{x}_\theta\) would be \(\frac{1}{2} \hbar^2 \sin^2(\eta) + \hbar \sin^2(\eta) \hat{\eta} + \frac{1}{2} \sin^2(\eta) \hat{\eta}^2\) which provides the exact diagonal elements. Therefore we have diagonalized the corresponding matrix numerically. For lower eigenvalue labels \(\nu\), both the eigenvalues and the eigenfunctions of the later ordering gave a worse approximation to those of the exact \(\hat{x}_\theta\) matrix than the ordering (37). In the semiclassical limit of high quantum numbers \(\nu\), the difference in the outcome for the two compared orderings practically disappeared as expected.

The form (37) of \(\hat{x}_\theta\) is the starting point of calculating its spectrum and its eigenfunctions analytically. The eigenvalue problem is stated as:

\[
\hat{x}_\theta | \xi_\nu \rangle = 2 \hbar \sin^2(\eta) \hat{\eta} | \xi_\nu \rangle = \xi_\nu | \xi_\nu \rangle.
\]

In angle representation and with \(\langle \theta | \xi_\nu \rangle = \psi_\nu(\theta)\), it can be written in the standard form of a Mathieu equation ([37], 20.1.1):

\[
\frac{d^2}{d \eta^2} \psi_\nu(\theta) + (a_\nu - 2q_\nu \cos 2\eta) \psi_\nu(\theta) = 0
\]

where

\[
a_\nu = 2q_\nu, \quad q_\nu = 2 \xi_\nu.
\]

It is an eigenvalue equation since \(\theta\) is an angle variable, and we are therefore looking for periodic solutions of the form:

\[
\psi_\nu(\theta) = \sum_{k=0}^\infty A^\nu_k \cos(2k\eta).
\]

If we define ([37], 20.2.13):

\[
V_n = (4 \xi - m^2)/(2 \xi)
\]
the eigenvalues \( \xi_v \) of (41) are given as the zeros of the following continued fraction ([37], 20.2.21)

\[
V_0 - \frac{1}{V_2 - \frac{1}{V_4 - \frac{1}{V_6 - \cdots}}} = 0.
\]

(45)

Since the zeros of (45) are discrete, so is the spectrum of \( \hat{x}_B \), and \( \nu \) can be chosen an integer to label the states. The discreteness of the spectrum of \( \hat{x}_B \) is a noteworthy result, since it is well known that the unrestricted \( \hat{x} \) operator has a continuous spectrum. Moreover, a countable basis does not necessarily guarantee a discrete spectrum as, e.g., shown in [38] for the case of the kicked rotor on resonance. The second column of Table 1 shows a list of the first ten zeros of (45). They can be compared with eigenvalues of the \( \hat{x}_B \) operator, which were obtained by diagonalizing \( \hat{x}_B \) in a basis of 1800 unperturbed \( |n> \) states (see first column of Table 1).

The zeros of (45), i.e., the eigenvalues \( \xi_v \) of (40) can also be obtained from the zeros of the following equation ([37], 20.2.30) which is valid for \( \xi_v \gg 1 \):

\[
0 = -8 \xi_v + 2w_v \sqrt{2 \xi_v - \frac{w_v^2 + 1}{w_v^2 + \frac{3w_v}{2}} - \frac{d_1}{d_2} - \frac{d_3}{d_4} - \frac{d_5}{d_6} - \cdots} = 1, 2, 3, \ldots
\]

(46)

where

\[
\begin{align*}
    d_1 &= 5 + \frac{34}{w_v^4} + \frac{9}{w_v^6} \\
    d_2 &= \frac{33}{w_v^2} + \frac{410}{w_v^4} + \frac{405}{w_v^6} \\
    d_3 &= \frac{63}{w_v^2} + \frac{1260}{w_v^4} + \frac{2943}{w_v^6} + \frac{486}{w_v^8} \\
    d_5 &= \frac{527}{w_v^2} + \frac{15617}{w_v^4} + \frac{69001}{w_v^6} + \frac{41607}{w_v^8} \\
\end{align*}
\]

(47)

and

\[
\begin{align*}
    w_v &= 4v + 1; \\
    \varphi_v &= 2 \xi_v w_v^4.
\end{align*}
\]

(48)

Equation (46) yields acceptable values for the semiclassical eigenvalues \( \xi_v \). The first 10 zeros of (46) are listed in the third column of Table 1. According to the regime of validity of (46), the accuracy improves for larger \( \nu \). At \( \nu = 10 \), e.g., it has reached 6%.

Since it is now shown that (41) has a discrete spectrum, we might also try direct Bohr-Sommerfeld quantization of \( \hat{x}_B \). We interpret \( x_B(n, \theta) = 2n^2 \sin^2 \eta(\theta) \) as a classical Hamilton function depending on the two conjugate variables \( n \) and \( \theta \). The quantized values \( \xi_v \) of \( x_B \) are then obtained by the quantization condition:

\[
\frac{1}{2\pi} \int \frac{n}{d} d\theta = \frac{1}{2\pi} \int \frac{2\xi}{d} d\theta = v + \frac{\alpha}{4}
\]

(49)

where \( \alpha \), the Maslov index [39], is equal to 1 since the \( x_B = \xi_v = \text{const.} \) trajectory has exactly one turning point (see Fig. 1b).

From (49) with (10d) we get:

\[
\xi_v = \frac{\pi^2}{8} (v + 1/4)^2.
\]

(50)

To leading order in \( \nu \), (46) also predicts a \( \nu^2 \) law for the eigenvalues \( \xi_v \). If we let \( \xi_v \sim \nu^2 \) in (46) and keep only the leading power in \( \nu \), we get an equation for \( \lambda \), which reads:

\[
1 = -4\lambda + 4\sqrt{2}\lambda^{1/2} - \frac{1}{8} \sqrt{2} \lambda^{-1/2} - \frac{5}{64} \lambda^{-1} - \frac{33\sqrt{2}}{1024} \lambda^{-3/2} + \frac{63}{2048} \lambda^{-2} - \frac{527\sqrt{2}}{32768} \lambda^{-5/2} - \cdots
\]

(51)

The solution of this equation is \( \lambda = 1.2802 \), which, taking into account the slow convergence of (51), compares very favorably with \( \pi^2/8 = 1.2337 \).

Since we want to understand the asymptotic behavior of the time dependent wave functions from Sect. II, we now investigate the semiclassical wave function (43). The expansion coefficients \( A_{2k}^{(n)} \) in (43) satisfy the recursion relation:

\[
2A_{2k}^{(n)} - A_{2(k+1)}^{(n)} = 0
\]

(2\( \xi_v \) - 2)\( \xi_v \)(2\( A_{2k}^{(n)} + A_{2(k+1)}^{(n)} \)) = 0

(4\( \xi_v \) - \( m^2 \))\( A_{2k}^{(n)} - 2\( \xi_v \)(\( A_{2k-2}^{(n)} + A_{2k+2}^{(n)} \)) = 0, \quad m \geq 3
\]

(52)

where we used \( a_v = 4\( \xi_v \) \) and \( q_v = 2\( \xi_v \) \) from (42).

In \( n \) representation, the states (43) are given by

\[
\langle n|v \rangle = \int_0^\pi \langle n|n \rangle \langle n|v \rangle d\theta = \sqrt{\frac{\pi}{2}} \int_0^\pi \cos n(\theta) \psi_v(\theta) d\theta = 4 \sqrt{\frac{2}{\pi}} \sum_{k=0}^\infty A_{2k}^{(n)} \int_0^{\pi/2} \cos n(2\eta - \sin 2\eta) \cos(2k\eta) \sin^2\eta d\eta.
\]

(53)

The integral in (53) can be calculated analytically and we obtain:

\[
\langle n|v \rangle = \sqrt{\frac{\pi}{2}} \sum_{k=1}^{\infty} k A_{2k}^{(n)} [J_{n-k}(\xi_v) - J_{n+k}(\xi_v)].
\]

(54)

For fixed \( v \), the coefficients \( A_{2k}^{(n)} \) oscillate up to \( k = 2v \) and decay exponentially for higher \( k \) values, as has been shown by numerical investigations. Therefore, requiring \( n \gg 2v \) ensures that, for all \( k \) values giving relevant contributions to the sum over \( k \) in (54), the
condition $n \gg k$ is fulfilled. An asymptotic expression for $J_{n-k}(n) - J_{n+k}(n)$ in the limit $n \to \infty$, can thus be obtained by applying the asymptotic expansion of Bessel functions whose order and argument are nearly equal (see [40], formula 8.42(7)). To leading order in $n$, the result is given by:

$$J_{n-k}(n) - J_{n+k}(n) \sim C_1 \frac{k}{n^{2/3}} + C_2 \left(\frac{k^3}{6} - \frac{k}{15}\right) \frac{1}{n^{5/3}}.$$  (55)

with constants $C_1$ and $C_2$. The exponential decay of the $A_{nk}^{(9)}$ amplitudes as a function of $k$ also guarantees the existence of the moments

$$M_k^{(9)} = \sum_{k=1}^{n} k^r A_{nk}^{(9)}.$$  (56)

It is easy to prove from the recurrence relations (52) that $M_k^{(9)}=0$. Substituting (55) in (54), we obtain:

$$\langle n | v \rangle \sim n^{-7/3}.$$  (57)

independent of $v$. Figure 3b shows a comparison of the exact $\langle n | v \rangle$ expansion coefficients of the fifteenth $\chi_9$-eigenstate (full line) with the fifteenth semiclassical state (54) (dashed line). The actual calculation of the semi classical state was carried out by diagonalization of (38) in a basis of 2500 states. This is equivalent to, but more convenient than summing up (54) (note the basis truncation effects in the "semiclassical" state in Fig. 3b). The structure of the two states is very similar. Both states show a powerlaw for $n < n_1^{(9)}$, oscillations for $n_1^{(9)} < n < n_2^{(9)}$ and a powerlaw for $n > n_2^{(9)}$. The agreement between the exact and the semiclassical state is nearly perfect in the oscillatory regime. There is a noticeable difference in the two powerlaw regimes. As is expected, the agreement between exact and semiclassical $\chi_9$ eigenstates improves when we proceed further towards the semiclassical limit by raising the quantum number $n$. Yet, the later onset of the smooth powerlaw behavior for high $n$ (see discussion of $n_2^{(9)}$ below) makes an extraction of powerlaw values from the numerically calculated eigenvectors less precise because of the basis limitation.

As mentioned above, the $\chi_9$-eigenfunctions show a characteristic drop at $n \approx n_1^{(9)}$ (see Fig. 3). This drop is easily explained. For a given $x$-state with eigenvalue $\xi_x$, the corresponding classical motion in the $(n, \theta)$ space is on the line $\xi_x = 2n^2 \sin^2 \eta(\theta)$ which has a turning point at $n = \sqrt{\xi_x} / 2$. The $n$ values with $n < n_1^{(9)}$ are classically forbidden. In semiclassical approximation we have $\xi_x \approx \frac{\pi^2}{8} (v + 1)^2$ and therefore $n_1^{(9)} = \frac{\pi}{4} (v + 1)$. This result accounts very well for the $n$ values where the sharp drop occurs in Fig. 3. For more examples compare Fig. 8 in [10]. We extracted $n_1^{(9)}$ for the first hundred $\chi_9$-eigenstates, which were obtained by direct diagonalization in a basis of 1000 states. Excellent agreement was obtained.

For $n > n_1^{(9)}$ the expansion coefficients $\langle n | v \rangle$ oscillate as a function of $n$ until the asymptotic region, characterized by the smooth powerlaw behavior, is reached. The last $n$ for which the coefficient $\langle n | v \rangle$ changes sign is calculated from the condition that the action integral $S = \int n \mathrm{d} \theta$ is exhausted up to one unit of $\hbar$, i.e., $S(n_2^{(9)}) = 2\pi(v - 3/4)$. From this implicit condition we get: $n_2^{(9)} \approx \frac{\pi}{4\sqrt{6}} (v + \frac{1}{2})^{3/2}$. This estimate, as can be confirmed with the help of Fig. 2a and Fig. 3, is in excellent agreement with the onset of smooth behavior extracted from numerically obtained $\chi_9$-eigenfunctions (see Fig. 2 and Fig. 8 in [10] for more numerical material).

IV. Discussion

In the previous sections we developed the scenario of a crossover of microwave driven hydrogen atoms from regular to chaotic to $x$ dominated motion as a function of principal quantum number $n$. It was argued that chaotic motion is obtained if $H_0$ and $V$ are of the same order of magnitude. With (10a) and (10d) this means: $1/2n^2 \approx 2n^2 \xi$ from which we obtain $n_{\text{chaos}} \approx (1/4\xi)^{1/2} = 14$ for the parameters of Fig. 1b. And indeed, $n_{\text{chaos}} = 14$ is roughly in the middle of the chaotic strip in Fig. 1b. $x$ motion takes over if $V$ outweighs $H_0$. In general it is hard to tell how much larger $V$ has to be in order to dominate over $H_0$. In Fig. 1b $x$ motion sets in at $n \approx 20$. At $n = 20$ and $\theta = \pi$, $V$ is about 4 times stronger than $H_0$. Thus, the results presented in Fig. 1 fit our intuitive understanding of an order $\to$ chaos $\to$ order transition as a function of $n$.

On a more fundamental level, we also obtained very detailed results on the localization properties of the quasi energy states of the one dimensional microwave driven $H$ atom. Based on detailed numerical calculations and a semiclassical analysis, we conclude that all quasi energy states $|x\rangle$ of the one dimensional driven $H$ atom are powerlaw localized in the regions (ii) and (iii), that is $\langle n | x \rangle \sim n^{-s}$, $s = 7/3$ for large $n$. Figure 2a and b give clear evidence for this fact. The powerlaw is explained to arise from the $x$ dominance at large $n$. The validity of this picture is underlined in Fig. 2a, which shows a quasi energy state localized in the large $n$ domain (full line) together with the $\chi_0$-eigenstate $|\psi^{(4)}\rangle$ (dashed line). The similarity between the two states is striking. Reviewing
the literature, there have been two attempts so far to address the question of the localization properties of the one dimensional driven H atom. Both attempts, like in our case, restrict the H atom to the set of bounded states. Bardsley et al. [29] arrived at a classification of quasi energy states into three types, which, similar to our notation, were called type I, II and III. Type I states in [29] correspond to the strongly localized states in region (i) associated with classically regular motion. Type II states were called "transitional" and the chaotic motion, according to [29] should be carried by Type III states. The seemingly irregular behavior of Type III states in [29], however, is not real. Since the authors of [29] worked in a basis of only 29 states, their Type III region reflects nothing but basis truncation errors. Thus, although [29] clearly brings out the classification of the quasi energy states into three regimes, our analysis shows that classically chaotic motion has to be identified with Type II states (= region (ii)) and Type III states have to be identified with x dominated motion (= region (iii)).

The localization properties of the quasi energy states were only addressed in a speculative way in [29]. It was conjectured that Type III states might be unnormalizable, a claim which on the basis of the above results can be clearly refuted.

The authors of [41] concentrate on the localization properties of quasi energy states in region (ii). They conclude that here the quasi energy states are exponentially localized in the photon number, i.e., the number of photons it takes to directly ionize a given \(|n\rangle\) state by multiphoton ionization. These results are supported by our analysis [28] as long as the localization properties of the quasi energy states are investigated for principal quantum numbers \(n\) which overlap with region (ii). Because of the finite number of photon states, region (iii) is effectively represented by at most a few photonic states which is not enough to analyze the asymptotic localization properties of quasi energy states.

The best studied localization model so far is the kicked rotor [24, 25]. In this model all the quasi energy states are believed to be exponentially localized in the rotational quantum number. The propagator in this case can be well approximated by a banded matrix. Therefore, it can be mapped to the well known Anderson model of localization in disordered solids [24, 25] and the exponential localization is due to the finite range hopping probabilities in this model. This is not the case in the present problem which displays long range hopping. The localization is due to a different mechanism which, as we have shown, results in a powerlaw instead of exponential localization.

V. Summary and conclusions

In this paper we demonstrated the existence of three dynamical regimes in the bound space projected dynamics of strongly driven H Rydberg atoms. The three regimes are strikingly apparent both in the classical as well as in the quantum mechanical version of driven H Rydberg atoms. The division into three regimes is also reflected in the structure of the quasi energy states. Although vastly different in appearance for small \(n\), all, except for the strongly \(n\) localized, quasi energy states decay asymptotically like \(n^{-7/3}\) for large \(n\). The localization exponent is independent of the driving frequency, so that H Rydberg wave functions, independently of the frequency regime, are always asymptotically powerlaw localized. Microwave experiments are currently conducted in the "high frequency" (\(\omega n_0^2 > 1\)) and the "low frequency" (\(\omega n_0^2 < 1\)) regime. In the high frequency regime, the onset of smooth powerlaw behavior occurs for \(n\) values which are not yet reachable with existing experimental set ups. In the "low frequency" regime, however, region (iii) can be probed experimentally. Scaling Fig. 1b to \(n_0 = 32\) (see [1]), the onset of the smooth powerlaw regime is predicted to occur at \(n \approx 150\). For stronger driving, the onset of regime (iii) occurs at even lower \(n\) values.

So far, our model does not include the continuum. It is possible that the continuum affects the details of the decay of the wavefunctions for large \(n\). Preliminary calculations [11], indeed, point to a more gentle decline of the wavefunctions in region (iii) without affecting in any way the existence of the three dynamical regimes.

It is a pleasure to thank D. Wintgen and J. Bellissard for helpful and stimulating discussions. This research was supported in part by the NSF under grant number CHE88-19436 and the Stiftung Volkswagenwerk.

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