A Wave Packet can be a Stationary State

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Abstract

We establish the existence of strongly localized wave packets tracing *without dispersion* the classical dynamics of a Rydberg electron in a circularly polarized microwave field over up to 10^6 periods of the driving field, which at the same time are single eigenstates of the atom dressed by the microwave field. These "single state wave packets" are shown to be robust towards small changes of the external field and can be prepared experimentally.

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For time-periodic systems, the Floquet theorem ensures that any solution of the Schrödinger equation can be expressed as a linear combination of elementary time periodic solutions, eigenstates of the Floquet Hamiltonian. A simple physical example is the interaction of an atom with a monochromatic electromagnetic wave: the Floquet eigenstates are here the dressed states of the atom in the field, the quasienergies of the Floquet Hamiltonian being the energy levels of the dressed atom [1]. The purpose of this letter is to show that, for such

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a system, there can be *one single eigenstate* of the atom dressed by the field - a stationary state of the Floquet Hamiltonian - which is a wave packet locked on the field frequency. The nonlinear interaction between the atom and the driving field naturally reassembles the electronic probability at a well defined position, in one distinct eigenstate which evolves like a classical object *without dispersion* (this is analogous, in a different context, to the propagation of solitons). No need any more for the conventional creation of a wave packet by superposition of several quantum eigenstates - the nonlinearity does all the job!

A first example of such a "single state wave packet" or "wave packet eigenstate" has been recently found [2, 3] in atomic Rydberg states driven by a strong linearly polarized microwave field. This new quantum object has been shown to follow the classical dynamics for more than 10^6 field cycles (or Kepler periods of the unperturbed Coulomb motion). A related phenomenon has been observed in the dynamics of a gaussian wave packet launched along a stable classical orbit in the nonlinear dynamics of Rydberg electrons driven by a circularly polarized microwave field [4]: this wave packet has been shown to be stable against dispersion for at least ten field cycles [4]. In this letter, we establish the connection between both phenomena: this wave packet is in fact supported by a single resonant-type state of the Floquet Hamiltonian, stable against ionization for more than 10^6 Kepler periods and strictly non dispersive.

We consider a hydrogen atom in a circularly polarized microwave field of frequency ω and amplitude F (in atomic units), restricted to the plane defined by the the driving field. In the rotating frame, one obtains a time-independent Hamiltonian [5, 6]

$$H = \frac{\mathbf{p}^2}{2} - \frac{1}{r} - Fx - \omega \ell_z, \tag{1}$$

with ℓ_z the angular momentum operator. For $F = 0$, the eigenstates of H are labeled by the principal quantum number $n = 0, 1, 2, \ldots$ and by the angular momentum quantum number $m = -n, \ldots, n$, with energies $E_{n,m} = -1/2(n+1/2)^2 - m\omega$. For arbitrary F, the energy levels of H are quasienergies of the corresponding Floquet (dressed) Hamiltonian. The eigenstates of H evolve, in the laboratory frame, periodically in time with the frequency of the driving field.

We now proceed by the numerical diagonalisation of H in a Sturmian basis, after a complex dilation [7]. This yields (quasi)energies, widths (ionization rate induced by the microwave field), and wavefunctions of the Floquet states [8]. These results of our *exact* numerical treatment of the problem can now be compared to those of ref. [4].

To find the wave packet eigenstate among thousands of eigenstates of H, we use the classical stability analysis of ref. [4]. The stable circular orbit (in the laboratory frame) is represented by a fixed point $(x_0, y_0 = 0)$ in the rotating frame, with x_0 given by:

$$\frac{1}{\omega^2 x_0^2} - \frac{F}{\omega^2} = x_0, \tag{2}$$

For the equilibrium to be stable, the dimensionless parameter

$$q = \frac{1}{\omega^2 x_0^3} \tag{3}$$

must fall into the intervall $8/9 < q < 1$ [4]. Harmonic approximation to the Hamiltonian around this point yields:

$$H_{\rm osc} = E_{\rm eq.p.} + \omega_+(a_+^\dagger a_+ + \frac{1}{2}) - \omega_-(a_-^\dagger a_- + \frac{1}{2}), \tag{4}$$

where [9]

$$E_{\rm eq.p.} = \frac{1-4q}{2q^{2/3}}\omega^{2/3} \tag{5}$$

is the minimum energy at (x_0, y_0). $(a_+^\dagger, a_+)$ and $(a_-^\dagger, a_-)$ are commuting sets of creation-annihilation operators for the normal modes ω_+ and ω_-, given by [9]

$$\omega_\pm = \sqrt{\frac{2-q \pm \sqrt{q(9q-8)}}{2}}\omega. \tag{6}$$

The energy of the ground state of $H_{\rm osc}$ is

$$E_0 = E_{\rm eq.p.} + \frac{\omega_+ - \omega_-}{2}. \tag{7}$$

Given E_0 as an approximation to the (quasi)energy of the *real* wave packet eigenstate of the dressed atom, we can now find the latter in the exact Floquet spectrum. For the sake of comparison with ref. [4], we use the optimum value of the stability parameter, $q = 0.9562$. In order to check the rôle of the quantum mechanical coarse graining of the classical dynamics, we performed the calculations for various values of the microwave frequency $\omega = 1/n^3$, with $n = 15$, 30, 60 and 120. The appropriate amplitudes of the microwave field follow via Eqs.(2) and (3): $F = -0.04442\omega^{4/3} = -0.04442/n^4$. Fig. 1 shows the probability densities obtained. Clearly, these stationary states of the atom dressed by the field are *wave packets* localized at the stable equilibrium position (x_0, y_0) in the rotating frame which, in the laboratory frame, rotate around the nucleus at the microwave frequency without dispersion. As n increases, the effective size of $\hbar$ decreases and so does the extension of the wave packet [2, 3]. Nontheless, even for the lowest value $n = 15$, this eigenstate of the atom in the field *exists* and *does not disperse.* In Fig. 1 (c), we use the values suggested in ref. [4] for $n = 60$, i.e. $\omega/2\pi = 31.8$ GHz and $F = 19.3$ V/cm, instead of the optimum values set by $q = 0.9562$ ($\omega/2\pi = 30.5$ GHz and $F = 17.6$ V/cm). Although they differ by few percents, the characteristic structures of the wave packet are unaffected, which shows its robustness with respect to small deviations from the optimal stability conditions. The lifetimes of the states shown in fig. 1 are $\tau \simeq 11$ μs ($n = 15$), 3 ns ($n = 30$), 11 μs ($n = 60$), and $\tau \geq 1$ ms for $n = 120$ (accuracy limited by double precision arithmetics). For $n = 15$ and $n = 120$, this corresponds to at least 10^6 Kepler periods of the wave packet around the nucleus, indicating an almost "eternal" life time of these two eigenstates. The shortest life time $\tau \simeq 3$ ns (for $n = 30$) still corresponds to approx. 1000 Kepler periods. For certain values of n, unharmonic corrections to $H_{\rm osc}$ destabilize the eigenstate, via avoided crossings with adjacent eigenstates of the quantum problem.

For example, the wave packet eigenstate in fig. 1(b) is, accidentally, almost degenerate with another, completely different Floquet state [9]. The induced mixing is manifest in the less regular probability density and strongly reduces τ. It can be shown [9] that the wave packets discussed can be expressed as a combination involving mainly circular states centered about a given n value.

There are other Floquet states localized in the vicinity of the stable equilibrium. The harmonic approximation, Eq. (4), predicts a double ladder of excited states along the normal modes ω_+ and ω_-. The energies of the two eigenstates of $H_{\rm osc}$ with a single quantum in either of the modes ω_+ or ω_- should be $E_0 \pm \omega_\pm$. We find the corresponding Floquet eigenstates, for $n = 120$, very close to the predicted energies. Their probability densities are plotted in Fig. 2. These are again localized single state wave packets, with almost eternal lifetimes. Both wavefunctions vanish at the equilibrium position, as does the first excited state of a harmonic oscillator. The normal modes completely entangle the 4 position-momentum coordinates, preventing the wavefunctions to separate either in local cartesian or polar coordinates. However, as immediately evident from Fig. 2, radial (resp. angular) excitation clearly dominates for one quantum in the ω_+ (resp. ω_-) mode.

Let us finally address possible experimental ways to prepare the single state wave packets in the laboratory. The direct optical resonant excitation from some low lying state is excluded since the wave packet is localized far from the nucleus. The adiabatic population transfer via a slow switching of the microwave is also inadequate because of the large number of very small avoided crossings (see below). Diabatic population is closest to state of the art microwave experiments [10] and we shall focus on this approach.

By diabatic population we understand assembling the wave packet by sufficiently rapid switching of the microwave field experienced by the atoms. This necessitates the knowledge of the zero field limit of the wave packet eigenstate via Eqs. (2)-(7). Our single state wave packet is the diabatic continuation of the circular state $|n, n>$ only if $\omega = 1/n^3$, with n an integer. For other values of the frequency, the wave packet exists in the presence of a sufficiently strong field but it does not evolve smoothly into a single state at vanishingly small field. It rather goes through a complicated series of large avoided crossings, losing progressively its identity [9].

Even if ω is properly chosen, the diabatic continuation of $| n, n >$ for nonvanishing field amplitudes encounters avoided crossings with other eigenstates which have to be crossed diabatically (sufficiently fast). It is the size of these avoided crossings which sets the time scale for sufficiently rapid switching of the microwave field. Fig. 3 shows the quasienergy difference (measured in units of the zero-field mean level spacing) between the wave packet eigenstate of the real system and the ground state of the harmonic approximation, as a function of the scaled amplitude $F_0 = Fn^4$ of the microwave field. Obviously, the harmonic approximation is excellent (differing by much less than the mean level spacing [9] from the exact value) for all values of F_0, except in the immediate vicinity of $F_0 \simeq 0.0215$ and $F_0 \simeq 0.0353$. There, the Floquet state originating from the initial circular state undergoes an avoided crossing with an adjacent state (the corresponding states of the harmonic approximation just cross). The two critical values of the field amplitude correspond to the classical $1:4$ (and $1:3$) resonances between the normal modes ω_+ and ω_- [9], and mark

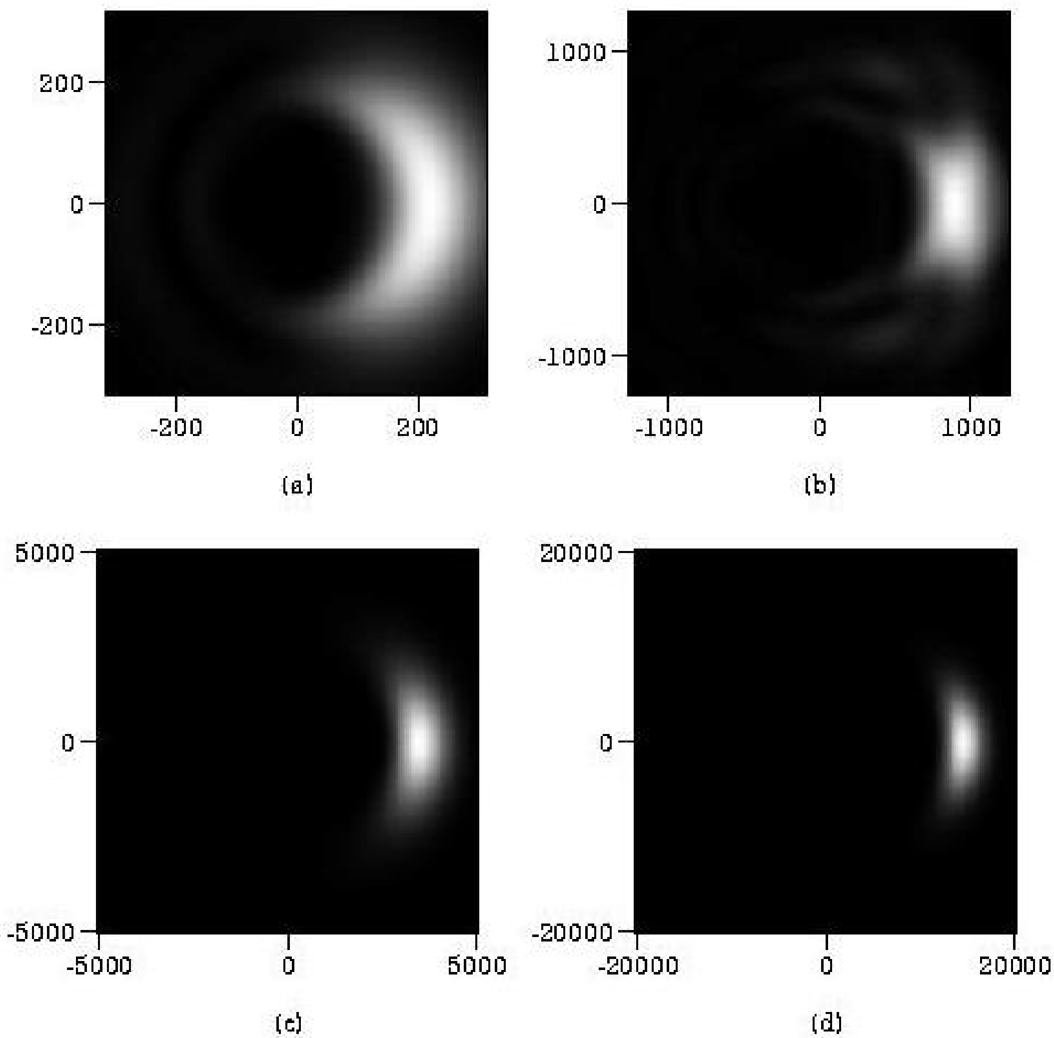

Figure 1: Probability densities of atomic hydrogen in a circularly polarized microwave field of frequency ω and amplitude F, in the rotating frame of the field. These are wave packet eigenstates of the Hamiltonian (1), localized near a classically stable equilibrium position. In the laboratory frame, these single state wave packets rotate around the nucleus with the microwave frequency and do not spread. (a) $n = 15$, $\omega/2\pi = 1.95$ THz, $F = 4516$ V/cm, lifetime $\tau \simeq 11$ μs, scale ± 312 a.u. from the nucleus (located at the center of the plot). (b) $n = 30$, $\omega/2\pi = 244$ GHz, $F = 282$ V/cm, $\tau \simeq 3$ ns, scale ± 1250 a.u. (c) $n = 60$, $\omega/2\pi = 31.8$ GHz, $F = 19.3$ V/cm, $\tau \simeq 11$ μs, scale ± 5000 a.u. (d) $n = 120$, $\omega/2\pi = 3.8$ GHz, $F = 1.1$ V/cm, $\tau \geq 1$ ms, scale ± 20000 a.u.

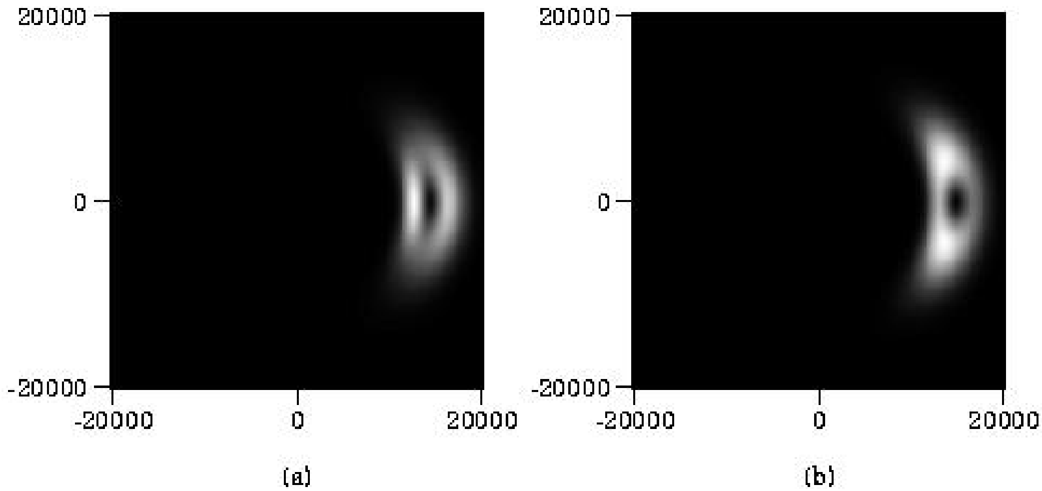

Figure 2: Probability densities corresponding to the first excited states of the local normal modes ω_+ (a) and ω_- (b), in the vicinity of the equilibrium position (scales as in Fig. 1d). Note the neat one-quantum excitation mainly along the radial (a) and angular directions (b), respectively, together with the central node, as expected from the harmonic approximation of the Hamiltonian.

the degeneracy of the ground state in the harmonic approximation with the states with one quantum in the ω_+ mode and 4 (resp. 3) quanta in the ω_- mode. The nonlinear coupling between the normal modes induced by the unharmonic corrections to the local potential lifts this degeneracy and causes the avoided crossings visible in fig. 3.

From fig. 3 we can now extract the order of magnitude of the *upper limit* for the switching time Δt of the microwave field in order to achieve diabatic population of the single state wave packet. If we want a minimum percentage P of the initial population to cross the energy gap ΔE between the anticrossing states, the Landau-Zener formula yields for the time scale [11]:

$$\Delta t \simeq -\frac{\ln P}{\Delta E}\frac{F_{\max}}{\Delta F}. \tag{8}$$

$F_{\max}$ is the maximum value of the field amplitude experienced by the atoms, and ΔF the width of the avoided crossing in F. For the cases shown in fig. 3, this estimation yields switching times of $\Delta t \simeq 10$ ns ($n = 60$), 100 ns ($n = 90$), and 0.8 μs ($n = 120$), respectively, for $P = 90\%$. Such values can be realized in current microwave experiments [10].

A possibility to indirectly prove the effective population of the wave packet eigenstate would consist in the experimental probing of its slow decay to the continuum, which is slowest as compared to the states encountered at the anticrossings. Field ionization spectroscopy [12] after the end of the microwave pulse should allow for an estimation of the population transfer to other Floquet states during the passage through the various avoided crossings. Note that a precise characterization of the initial (circular) state [12] the atoms are prepared in is *crucial* for the unambiguous identification of the wave packet eigenstate,

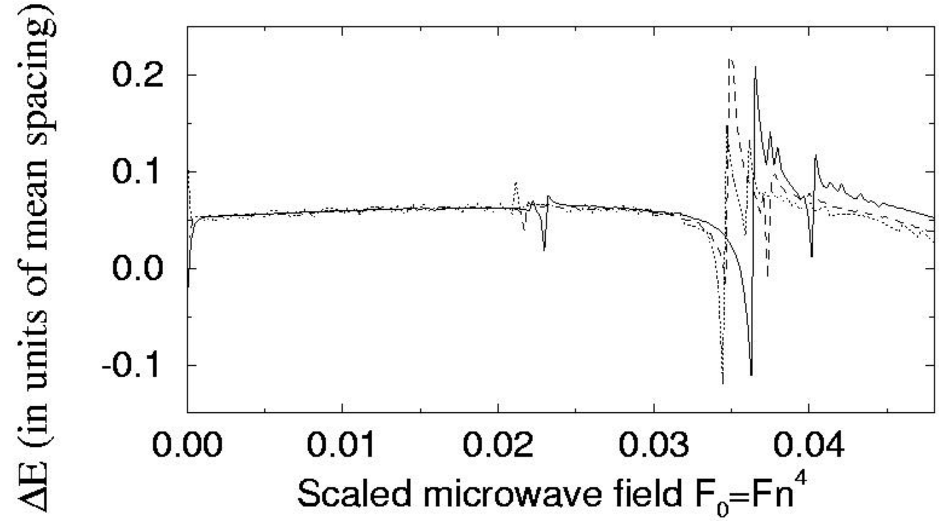

Figure 3: Difference ΔE between the energy of the exact wave packet eigenstate of H (eq. (1)) and the energy deduced from the harmonic approximation of the Hamiltonian of the Rydberg electron in the microwave field, in the vicinity of the stable equilibrium position (Eq. (7)). ΔE is plotted as a function of the scaled microwave amplitude $F_0 = Fn^4$, at fixed frequency $\omega = 1/n^3$. $n = 60$ (full curve), $n = 90$ (dashed curve), and $n = 120$ (dotted curve).

since there are other states with comparable lifetimes but with completely different spatiotemporal localization properties [2, 3, 9]. The robustness of the wave packet eigenstate ensures that small experimental imperfections, such as slight deviations from circular polarization of the microwave should not be important. Furthermore, due to the maximum overlap of the single state wave packet with circular states, which do not probe the Coulomb singularity, the experiment could also be performed on Rydberg states of non-hydrogenic atomic species.

Finally, the existence of the third dimension z perpendicular to the microwave field should not be a problem: indeed, the fixed point (x_0, y_0) in the rotating frame lies in the $z = 0$ plane and is classically stable (the Coulomb force along z is attractive). Consequently, non dispersive wave packets with small extension along z should also exist in a “real” 3d hydrogen atom in a circularly polarized microwave field. Their properties (lifetimes, excitation mechanism...) should be essentially the same than in 2d, which opens the way to their experimental observation.

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