Chaotic enhancement of hydrogen atoms excitation in magnetic and microwave fields

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Abstract

We numerically investigate multiphoton ionization of excited hydrogen atoms in magnetic and microwave fields when up to $N_I = 600$ photons are required for ionization. The analytical estimates for the quantum localization length in the classically chaotic regime are in agreement with numerical data. The excitation is much stronger as compared to the case with microwave field only due to the chaotic structure of eigenstates in magnetic field.

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In 1982 Shushkov and Flambaum discussed the effect of weak interaction enhancement due to a complex structure of ergodic eigenfunctions in nuclei. The basic idea of this effect is that in complex systems an eigenfunction, represented in some basis, has a large number $M$ of randomly fluctuating components so that their typical value is $1/\sqrt{M}$. Due to this, the matrix elements for interparticle interaction are $V_{\text{int}} \sim 1/\sqrt{M}$ while the distance between mixed levels is $\Delta E \sim 1/M$. As a result, according to the perturbation theory, the admixture factor $\eta$ is strongly enhanced: $\eta \sim V_{\text{int}}/\Delta E \sim \sqrt{M}$ as compared to the case in which eigenfunctions have only few components ($M \sim 1$). This effect was investigated and well confirmed in experiments with weak interaction enhancement for scattering of polarized neutrons on nuclei. Recently a similar effect of interparticle interaction enhancement was discussed for two interacting particles in disordered solid state systems. Here, a short range interaction produces a strong enhancement of the localization length leading to a qualitative change of physical properties. This shows that the effect is quite general and can take place in different systems.

In this Letter we investigate the possibility of similar enhancement in atomic physics for atoms interacting with electromagnetic fields. Such process becomes especially interesting for highly excited atoms (hydrogen or Rydberg atoms) in microwave fields where absorption of many photons is necessary in order to ionize electrons. Until now this problem was studied only in the case in which the electron dynamics, in absence of microwave field, is integrable. In this case strong ionization is possible due to onset of chaos at sufficiently strong field intensity. As it is known, above the classical chaos border ionization proceeds in a diffusive way and quantum interference effects can lead to localization of this diffusion and thus suppress ionization.

A quite different situation, which was never studied neither numerically nor experimentally, appears when the electron’s motion in the atom is already chaotic in the absence of microwave field. An interesting example of such situation is an hydrogen atom in a strong static magnetic field. The properties of such atoms have been extensively studied in the last decade and it has been shown that the eigenfunctions are chaotic, and that several
properties of the system can be described by Random Matrix Theory. Due to that one can expect that the interaction of such an atom with a microwave field will be strongly enhanced so that the localization length will become much larger than the corresponding one in the absence of magnetic fields. As a result, the quantum delocalization border, which determines the ionization threshold, will be strongly decreased.

The investigation of classical dynamics and some preliminary estimates for the quantum localization length in such a case have been given in a recent paper [6]. Here we discuss the quantum dynamics and present the results of numerical simulations which confirm the chaotic enhancement of quantum excitation as compared to the case without magnetic field. Our studies also show a number of interesting features which arise in this model in the adiabatic regime when the microwave frequency is much smaller than the Kepler frequency.

We consider the case in which the electric and magnetic fields are parallel. In this case the magnetic quantum number \( m \) is an exact integral of motion and here we set \( m = 0 \). The Hamiltonian writes

\[
H = \frac{p_z^2}{2} + \frac{p_\rho^2}{2} + \frac{\omega_L^2 \rho^2}{8} - \frac{1}{\sqrt{z^2 + \rho^2}} + \epsilon z \cos(\omega t),
\]

where \( \omega_L = B/c = B(T)/B_0 \) is the cyclotron frequency, \( B_0 = 2.35 \times 10^5 \text{T} \), \( \epsilon \) and \( \omega \) are the field strength and frequency respectively (atomic units are used). As it is known [4][5], in the absence of microwave field, the classical motion becomes chaotic for \( \omega_L n_0^3 \gtrsim 1 \) and no visible islands of stability are present for \( \omega_L n_0^3 \approx 9 \). For \( \omega_L n_0^3 = 3 \) some islands of stability exist but their size is small.

The turn on of microwave field leads to diffusive energy growth with classical diffusion rate per unit time \( D_B = (\Delta E)^2/\Delta t \). The dependence of \( D_B \) on parameters \( \epsilon, \omega \) has been found in [6]: \( D_B/D_0 \approx \chi_1 \omega_0^2 \) (\( \omega_0 \ll 1 \)), \( D_B/D_0 \approx \chi_2/\omega_0^{4/3} \) (\( \omega_0 \gg 1 \)), where \( \omega_0 = \omega n_0^3 \), \( D_0 = \epsilon^2 n_0/2 \) is the diffusion rate in the chaotic regime for \( B = 0 \) and \( \omega_0 = 1 \) and \( \chi_1, \chi_2 \) are two constants, weakly dependent on magnetic field (numerically, \( \chi_1 \approx 18 \), \( \chi_2 \approx 2 \) at \( \omega_L n_0^3 = 9.2 \) and \( \chi_1 \approx 25 \), \( \chi_2 \approx 1 \) at \( \omega_L n_0^3 = 3 \)). The above estimates for \( D_B \) give the asymptotic behavior of the diffusion rate for very small and very large \( \omega_0 \), while the actual
values of $D_B$ were determined from numerical simulations of the classical problem.

In the quantum case the interference effects can lead to localization of this diffusion. The localization length in number of photons $\ell_B$ is proportional to the one–photon transition rate $\Gamma$ and to the density of states $\rho_B$ coupled by these transitions [5]: $\ell_B \sim \Gamma \rho_B$. The transition rate $\Gamma$ can be derived from the classical diffusion rate: $\Gamma \approx D_B/\omega_0^2$. We recall that for the case $B = 0$ the localization length $\ell_\phi$ at $\omega_0 = 1$ is $\ell_\phi = 3.3\epsilon_0^2 n_0^2 \sim D_0 n_0^6 \rho_0$ [7], where $\rho_0 = n_0^3$ is the density of states and $\epsilon_0 = \epsilon n_0^4$. Due to Coulomb degeneracy and to the existence of an additional approximate integral of motion [7] the density $\rho_0$ is $n_0$ times smaller than the number of levels in one unit energy interval. As a result [3]

$$\ell_B = \ell_\phi \frac{D_B}{D_0 \omega_0^2} \frac{\rho_B}{\rho_0},$$

where it is assumed $\ell_B > 1$ and $\omega \rho_B > 1$. According to our quantum data $\rho_B/\rho_0 \approx n_0/(\omega_L n_0^3)$ for $\omega_L n_0^3 > 1$. More exactly $\rho_B/\rho_0 = 0.34 n_0$ (for $\omega_L n_0^3 = 3$, $n_0 = 60$) and $\rho_B/\rho_0 = 0.14 n_0$ (for $\omega_L n_0^3 = 9.2$, $n_0 = 60$). The dependence $\rho_B \sim 1/\omega_L$ is due to the oscillatory type behavior in $\rho$ direction in (1). The number of photons required for ionization is $N_I = n_0/2\omega_0$ and therefore for $\ell_B \ll N_I$ eigenfunctions are exponentially localized in the number of photons $N_\phi$, namely $\psi_N \sim \exp(-|N_\phi|/\ell_B)$.

The value of the localization length $\ell_B$ is strongly enhanced compared to the length $\ell_\phi = 3.3\epsilon_0^2 n_0^2/\omega_0^{10/3}$ at $B = 0$ and $\omega_0 > 1$. The enhancement factor $\ell_B/\ell_\phi \approx \chi_2 \rho_B/\rho_0 \approx \chi_2 n_0/(\omega_L n_0^3) \gg 1$ is proportional to the initially excited state $n_0$. In fact in the presence of a magnetic field there is no additional integral of motion [7] and the number of components in the eigenfunctions is increased by a factor $M = \rho_B/\rho_0$. As a result the admixture factor $\eta$ is also enhanced, namely $\eta^2 \sim M$ similarly to the enhancement of localization length in disordered solid state models with two particles [2] ($\ell_B/\ell_\phi \sim \eta^2 \sim M$).

The condition $\ell_B = N_I$ gives the delocalization border $\epsilon_q$ above which quantum excitation is close to the classical one (both for $\omega_0 < 1$ and $\omega_0 \geq 1$):

$$\epsilon_0 > \epsilon_q = \frac{1}{n_0} \sqrt{\frac{D_0 \omega_0^2}{6.6 D_B \rho_B \omega_0}}.$$
For $\omega_0 \geq 1$ this value is approximately by the factor $(3/n_0)^{1/2}$ below the delocalization border in microwave field only ($B = 0$) where $\epsilon_{q0} \approx \omega_0^{7/6}/\sqrt{6.6n_0}$. For $\omega_0 \ll 1$ the border is $\epsilon_q = (\omega_L/6.6\chi_1\omega)^{1/2}/n_0$.

In order to check the above estimates (eqs. (2) and (3)) we analyzed the quantum dynamics following the wave packet evolution in the eigenstate basis at $\epsilon = 0$. Initially only one eigenstate is excited with eigenenergy $E_{\lambda_0} \approx E_0 = -1/2n_0^2$ and $n_0 = 60$. In our computations we used a total number of eigenstates up to 800 and the evolution was followed up to time $\tau = 200$ microwave periods. The parameters were varied in the intervals $0.05 \leq \omega_0 \leq 3$, $0.002 \leq \epsilon_0 \leq 0.02$ for $\omega_Ln_0^3 = 3$ and 9.2. For this parameter range, the number of photons $N_I = n_0/2\omega_0$ required for ionization varies in the interval $10 \leq N_I \leq 600$. The probability distribution $f_\lambda$ over the eigenstates at $\epsilon = 0$ is shown in figs. 1, 2 as a function of the number of absorbed photons $N_\phi = (E_\lambda - E_0)/\omega$. In order to suppress fluctuations this probability was averaged over $10 - 20$ microwave periods. For the comparison with classical results we also determined the probability $f_N$ in each one–photon interval around integer values of $N_\phi$. The classical distribution was obtained by solution of Newton equations with up to $5 \times 10^3$ classical trajectories and was normalized to one–photon interval. Initially the trajectories were distributed microcanonically on the energy surface at energy $E_0$.

The typical results in the localized regime are presented in fig. 1. Here the distribution reaches its stationary state with a well localized exponential profile. The least square fit with $f_N \sim \exp(-2N_\phi/\ell_BN)$ for $N_\phi \geq 0$ allows to determine the numerical value of the localization length $\ell_BN$ which turns out to be in good agreement with theoretical estimate (eq. (2)) and is strikingly enhanced compared to the case of zero magnetic field. The plateau which appears in fig. 1b for $N_\phi > 130$ is related to the finite size of the basis and to the fact that, according to eq. (2), the localization length is non homogeneous on high levels ($\ell_B \sim n_0^{11} \sim (N_I - N_\phi)^{-11/2}$ for $\omega_0 \ll 1$).

In fig. 2 the distributions in the delocalized case are shown for $\omega_0 = 1$ (fig. 2a) and $\omega_0 = 0.1$ (fig. 2b). The delocalization borders in these cases, $\epsilon_q = 0.016$ (fig. 2a) and
\( \epsilon_q = 0.014 \), (fig. 2b) are below the field peak value \( \epsilon_0 = 0.02 \). The numerical results show a good agreement between classical and quantum distributions in this regime. Even if at \( \epsilon_0 = 0.02 \) the dynamics starts to be chaotic also at zero magnetic field, the excitation at \( \omega_L n_0^3 = 3 \) is much stronger due to the chaotic enhancement of electron’s interaction with the microwave field. For example, the increase of \( \langle (\Delta N_\phi)^2 \rangle \) after 50 microwave periods is approximately 55 for the case of fig. 2a while at \( B = 0 \) it is only 6.

In order to check the theoretical predictions for the photonic localization length \( \ell_B \) we analyzed different probability distributions in the localized regime for \( 0.05 \leq \omega_0 \leq 3 \) at \( \omega_L n_0^3 = 3 \) and \( \omega_L n_0^3 = 9.2 \). The comparison of the numerically obtained lengths \( \ell_{BN} \) with the theoretical estimate eq. (2) is presented in fig. 3. Without any fitting parameter the theoretical line demonstrates the fairly good agreement with numerical data. Indeed the average value of the ratio \( R = \langle \ell_{BN}/\ell_B \rangle = 0.81 \pm 0.34 \), where the average is over all values \( \ell_B > 1 \). The separate averaging over the cases with \( \omega_0 \geq 1 \) and \( \omega_0 < 1 \) gives \( R_1 = 0.98 \pm 0.30 \) and \( R_2 = 0.70 \pm 0.26 \) respectively.

In spite of the good agreement between theoretical predictions and numerical data we would like to stress that a deeper investigation of the problem is required. Especially unusual is the regime \( \omega_0 < 1 \), which has not been studied up to now from the viewpoint of dynamical localization. A number of new questions appear in this regime. For example for \( \omega_0 > 1 \) a chain of one–photon transitions is clearly seen in the quantum localized distribution (fig. 1a) while for \( \omega_0 < 1 \) the structure is not visible even though \( \omega_\rho B > 1 \) (fig. 1b).

Another interesting question in this adiabatic regime \( \omega_0 \ll 1 \) is connected with the possibility of analyzing the problem in the instantaneous time basis. In this basis the Hamiltonian takes the form \( H(t) = H_0(t) + \partial S/\partial t \), where \( H_0 \) is the Hamiltonian (1) at a given moment of time while \( \partial S/\partial t \) describes the transitions due to the field’s variation with time \( (S \) is the action of the Hamiltonian (1) in which time is considered as a parameter). The term \( \partial S/\partial t \) can be estimated as \( \partial S/\partial t \sim \epsilon \omega \sin(\omega t) 2\pi n^3 z \sim \epsilon \omega n^5 \) (see also [9]). It describes the transitions between instant time levels of the Hamiltonian (1), the amplitude of which can be estimated as \( V_{eff} \sim \epsilon \omega n^5/\sqrt{n} \). The factor \( \sqrt{n} \) in the denominator appears
due to the chaotic structure of eigenstates which leads to a smearing of $\partial S/\partial t$ over the $n$ states which contribute to the eigenfunctions inside an atomic shell (we assume $\omega_L \sim 1/n_0^3$). Since the distance between levels is $\delta E \sim 1/\rho_B \sim n_0^{-4}$ it seems that mixing between instant levels is possible only if $V_{eff} > \delta E$, giving $\epsilon_0 \omega_0 n_0^{3/2} > 1$. This adiabatic condition is more restrictive than the standard $\ell_B > 1$ ($\epsilon_0 n_0^{3/2} > 1$). However the numerical results (fig. 3) confirm our estimate (2). For a possible explanation of this discrepancy one may argue that the distance between coupled quasi-energy levels is $\delta E_\omega \sim \omega/n$ and then the condition $V_{eff} > \delta E_\omega$ gives $\ell_B > 1$ in agreement with the estimate (2). Another possible reason is that in the instant time basis the levels are moving with time and can therefore intersect each other giving $\delta E = 0$.

In conclusion our numerical investigations confirm the theoretical estimates for the photonic localization length (2) both for $\omega_0 \geq 1$ and $\omega_0 < 1$. Due to the chaotic structure of the eigenstates the quantum delocalization border is strongly lowered compared to the case with microwave field only. Since for $\omega_0 \ll 1$ a much larger number of photons is required for ionization ($N_I = 300$ in figs. 1b, 2b) experimental observation of localization and verification of theoretical predictions should be more easily feasible in laboratory experiments.
FIGURES

FIG. 1. Probability distribution as a function of photon number $N_\phi$. Quantum distribution $f_\lambda$ over the eigenbasis at $\epsilon = 0$ (full line); quantum probability in one–photon interval $f_N$ (circles); classical distribution in one–photon interval (dashed line). The straight line shows the fit for the exponential decay.

(a) $n_0 = 60$, $\omega_0 = 1$, $\omega_L n_0^3 = 3$, $\epsilon_0 = 0.005$, $\ell_{BN} = 3.6$, $\ell_B = 3$, $180 \leq \tau \leq 200$, $D_B/D_0 = 0.49$.

(b) $n_0 = 60$, $\omega_0 = 0.1$, $\omega_L n_0^3 = 3$, $\epsilon_0 = 0.005$, $\ell_{BN} = 29.5$, $\ell_B = 37.5$, $180 \leq \tau \leq 200$, $D_B/D_0 = 0.062$.

FIG. 2. Same as in fig. [1] but in the delocalized regime, with $\epsilon_0 = 0.02 > \epsilon_q \approx 0.015$, and $40 \leq \tau \leq 50$. The classical (dashed line) and quantum (circles) distributions in one–photon interval are close to each other.

FIG. 3. The numerically computed localization length $\ell_{BN}$ versus the theoretical estimate $\ell_B$ eq. (8) for $\omega_L n_0^3 = 3$, $\omega_0 \geq 1$ (full circles), $\omega_L n_0^3 = 3$, $\omega_0 < 1$ (full triangles), $\omega_L n_0^3 = 9.2$, $\omega_0 \geq 1$ (open circles), $\omega_L n_0^3 = 9.2$, $\omega_0 < 1$ (open triangles). The error bars obtained from least square fits of the localized distributions are also shown. The straight line corresponds to $\ell_{BN} = \ell_B$. 

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