Chaotic enhancement of hydrogen-atom excitation in magnetic and microwave fields

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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 than the case with microwave field only due to the chaotic structure of eigenstates in a magnetic field. [S1050-2947(97)03710-4]

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In 1982 Shushkov and Flambaum [1] 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 $1/\sqrt{M}$. Because of this, the matrix elements for interparticle interaction are $V_{int} \sim 1/\sqrt{M}$, while the distance between mixed levels is $\Delta E \sim 1/M$. As a result, according to the perturbation theory, the admixture factor η is strongly enhanced: $\eta \sim V_{int} / \Delta E \sim \sqrt{M}$ as compared to the case in which eigenfunctions have only a few components $(M \sim 1)$. This effect was investigated and confirmed in experiments with weak interaction enhancement for scattering of polarized neutrons on nuclei [1]. Recently, a similar effect of interparticle interaction enhancement was discussed for two interacting particles in disordered solid-state systems [2]. Here a shortrange 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 paper we investigate the possibility of similar enhancement in atomic physics for atoms interacting with electromagnetic fields. Such a 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 the absence of microwave field, is integrable [3]. In this case strong ionization is possible due to the 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 either numerically or experimentally, appears when the electron's motion in the atom is already chaotic in the absence of a microwave field. An interesting example of such a situation is a hydrogen atom in a strong static magnetic field. The properties of such atoms have been studied extensively in the past decade [4,5] and it has been shown that the eigenfunctions are chaotic and several properties of the system can be described by random matrix theory. Thus 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 that confirm the chaotic enhancement of quantum excitation as compared to the case without a magnetic field. Our studies also show a number of interesting features that 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 is

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

where $\omega_L = B/c = B(T)/B_0$ is the cyclotron frequency, $B_0 = 2.35 \times 10^5$ T, and ϵ and ω are the field strength and frequency, respectively (atomic units are used). As it is known [4,5], in the absence of a microwave field, the classical motion becomes chaotic for $\omega_L n_0^3 \ge 1$ and no visible islands of

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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 a classical diffusion rate per unit time $D_B = (\Delta E)^2 / \Delta t$. The dependence of D_B on parameters ϵ, ω has been found in [6]: $D_B / D_0 \approx \chi_1 \omega_0^2$ ($\omega_0 \ll 1$), $D_B / D_0 \approx \chi_2 / \omega_0^{4/3}$ ($\omega_0 \ge 1$), 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 χ_1, χ_2 are two constants, weakly dependent on the 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 ω_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 [6,7]. The localization length measured in the number of photons ℓ_B is proportional to the one-photon transition rate Γ and to the density of states ρ_B coupled by these transitions [8]: $\ell_B \sim \Gamma \rho_B$. The transition rate Γ can be derived from the classical diffusion rate: $\Gamma \approx D_B/\omega^2$. We recall that for the case B = 0 the localization length ℓ_{ϕ} 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 the existence of an additional approximate integral of motion [7], the density ρ_0 is n_0 times smaller than the number of levels in one unit energy interval. As a result [6],

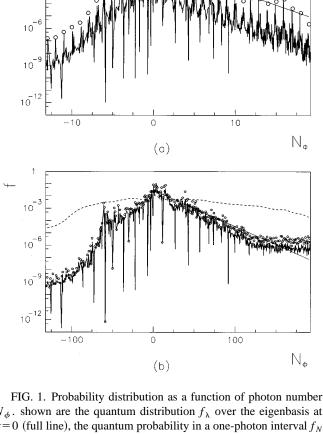
$$\ell_B = \ell_{\phi} \frac{D_B \rho_B}{D_0 \omega_0^2 \rho_0},\tag{2}$$

where it is assumed that $\ell_B > 1$ 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 the ρ direction in Eq. (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_{ϕ} , namely, $\psi_N \sim \exp(-|N_{\phi}|/\ell_B)$.

The value of the localization length ℓ_B is strongly enhanced compared to the length $\ell_{\phi\omega}=3.3\epsilon_0^2 n_0^2/\omega_0^{10/3}$ at B=0 and $\omega_0>1$. The enhancement factor $\ell_B/\ell_{\phi\omega}\approx\chi_2\rho_B/\rho_0\approx\chi_2n_0/\omega_Ln_0^3\geq 1$ 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 η is also enhanced, namely, $\eta^2 \sim M$, similarly to the enhancement of the localization length in disordered solid-state models with two particles [2] $(\ell_B/\ell_{\phi\omega} \sim \eta^2 \sim M)$.

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

$$\epsilon_0 > \epsilon_q = \frac{1}{n_0} \sqrt{\frac{D_0 \omega_0^2}{6.6 D_B} \frac{\rho_0 n_0}{\rho_B \omega_0}}.$$
 (3)



*N*_{ϕ} shown are the quantum distribution as a function of photon number N_{ϕ} , shown are the quantum distribution f_{λ} over the eigenbasis at $\epsilon = 0$ (full line), the quantum probability in a one-photon interval f_N (circles), and the classical distribution in a one-photon interval (dashed line). The straight line shows the fit for the exponential decay. (a) $n_0 = 60$, $\omega_0 = 1$, $\omega_L n_0^3 = 3$, $\epsilon_0 = 0.005$, $\ell_{BN} = 3.6$, $\ell_B = 3$, $180 \le \tau \le 200$, and $D_B/D_0 = 0.49$. (b) $n_0 = 60$, $\omega_0 = 0.1$, $\omega_L n_0^3 = 3$, $\epsilon_0 = 0.005$, $\ell_{BN} = 29.5$, $\ell_B = 37.5$, $180 \le \tau \le 200$, and $D_B/D_0 = 0.062$.

For $\omega_0 \ge 1$ this value is approximately by the factor $(3/n_0)^{1/2}$ below the delocalization border in the microwave field only (B=0), where $\epsilon_{q0} \approx \omega_0^{7/6} / \sqrt{6.6n_0}$. For $\omega_0 \le 1$ 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 wavepacket 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 $0.05 \le \omega_0 \le 3$, $0.002 \le \epsilon_0 \le 0.02$ for $\omega_L n_0^3 = 3$ 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 $10 \le N_I \le 600$. The probability distribution f_{λ} over the eigenstates at $\epsilon = 0$ is shown in Figs. 1 and 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_{ϕ} . The classical distribution was obtained by

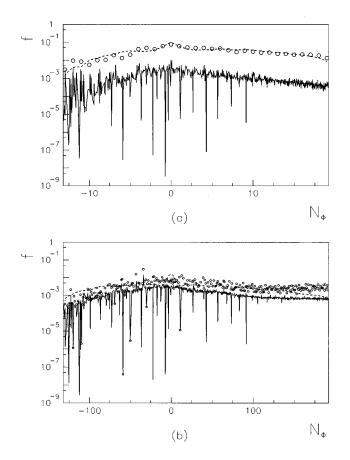


FIG. 2. Same as in Fig. 1, but in the delocalized regime, with $\epsilon_0 = 0.02 > \epsilon_q \approx 0.015$, and $40 \le \tau \le 50$. The classical (dashed line) and quantum (circles) distributions in one-photon interval are close to each other.

solution of Newton equations with up to 5×10^3 classical trajectories and was normalized to one-photon intervals. 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-squares fit with $f_N \sim \exp(-2N_{\phi}/\ell_{BN})$ for $N_{\phi} \ge 0$ allows one to determine the numerical value of the localization length ℓ_{BN} , which turns out to be in good agreement with the theoretical estimate [Eq. (2)] and is strikingly enhanced compared to the case of zero magnetic field. The plateau that appears in Fig. 1(b) for $N_{\phi} \ge 130$ is related to the finite size of the basis and to the fact that, according to Eq. (2), the localization length is nonhomogeneous 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. 2(a)] and $\omega_0 = 0.1$ [Fig. 2(b)]. The delocalization borders in these cases, $\epsilon_q = 0.016$ [Fig. 2(a)] and $\epsilon_q = 0.014$ [Fig. 2(b)], are below the field peak value $\epsilon_0 = 0.02$. The numerical results show 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 the 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

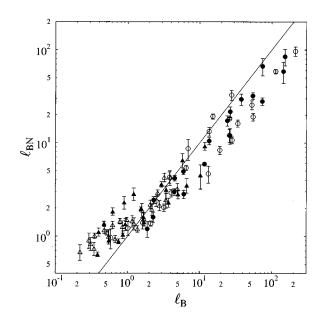


FIG. 3. Numerically computed localization length ℓ_{BN} versus the theoretical estimate ℓ_B Eq. (2) for $\omega_L n_0^3 = 3$, $\omega_0 < 1$ (full circles); $\omega_L n_0^3 = 3$, $\omega_0 \ge 1$ (full triangles); $\omega_L n_0^3 = 9.2$, $\omega_0 < 1$ (open circles); and $\omega_L n_0^3 = 9.2$, $\omega_0 \ge 1$ (open triangles). The error bars obtained from least-squares fits of the localized distributions are also shown. The straight line corresponds to $\ell_{BN} = \ell_B$.

for the case of Fig. 2(a), while at B = 0 it is only 6.

In order to check the theoretical predictions for the photonic localization length ℓ_B we analyzed different probability distributions in the localized regime for $0.05 \le \omega_0 \le 3$ at $\omega_L n_0^3 = 3$ and $\omega_L n_0^3 = 9.2$. The comparison of the numerically obtained lengths ℓ_{BN} with the theoretical estimate (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 $\omega_0 \ge 1$ 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. 1(a)], while for $\omega_0 < 1$ the structure is not visible even though $\omega \rho_B > 1$ [Fig. 1(b)].

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 that 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 quasienergy 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

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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) for both $\omega_0 \ge 1$ and $\omega_0 < 1$. Due to the chaotic structure of the eigenstates, the quantum delocalization border is strongly lowered compared to the case with a microwave field only. Since for $\omega_0 \ll 1$ a much larger number of photons is required for ionization [$N_I = 300$ in Figs. 1(b) and 2(b)], experimental observation of localization and verification of theoretical predictions should be more easily feasible in laboratory experiments.

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