Dynamical localization: Hydrogen atoms in magnetic and microwave fields

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We show that dynamical localization for excited hydrogen atoms in magnetic and microwave fields takes place at quite low microwave frequency ($\omega n^3 \ll 1$). Estimates of the localization length are given for different parameter regimes, showing that the quantum delocalization border drops significantly as compared to the case of zero magnetic field. This opens up broad possibilities for laboratory investigations. [S1050-2947(97)05102-0]

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Quantum-dynamical localization is one of the most interesting phenomena within the so-called field of "quantum chaos" [1]. This phenomenon, which consists in the quantum suppression of classically chaotic diffusive process, was discovered long ago [2], and has also been observed in several laboratory experiments [3-7]. Even though experimental results are in satisfactory agreement with theoretical predictions, the range of parameters over which quantum localization has been observed is still quite narrow. For example, in experiments performed on hydrogen and Rydberg atoms in microwave fields [3-5], in order to observe localization of the quantum probability distribution around the initially excited state n_0 , it is necessary that the localization length ℓ_{ϕ} of the distribution, measured in number of photons, be smaller than the number N_I of photons required for ionization. Such a condition imposes severe experimental restrictions. Indeed, $N_I = (2n_0^2\omega)^{-1} = n_0/2\omega_0$, where ω is the microwave field frequency and $\omega_0 = \omega n_0^3$ is the rescaled frequency; therefore, in order to increase N_I it is either necessary to increase the initially excited principal quantum number n_0 , or to decrease the rescaled frequency ω_0 . On the other hand, in real experiments $n_0 \leq 100$ and the additional condition $\omega_0 > 1$ must be verified if the system is to be found within the classically diffusive region (for sufficiently high field intensity ϵ). In practice, one typically obtains $N_I \approx 20$.

An interesting possibility for increasing N_I , thus allowing a better numerical and experimental analysis of dynamical localization, would be the consideration of a hydrogen atom within superimposed magnetic and microwave fields. Indeed, such a model, for a sufficiently strong magnetic field, displays classical chaotic dynamics even in the absence of the microwave field [8,9]. When the microwave field is turned on, this preexisting chaos immediately leads to the onset of classical diffusive energy excitation, even when the microwave field intensity ϵ goes to zero. Such excitation takes place even when $\omega_0 < 1$, therefore the quantity $N_I = n_0/2\omega_0$ can be significantly increased.

Quantum effects may lead to localization of classical diffusion, hence the critical microwave field intensity required for ionization or the so-called quantum ionization border will be determined by the condition $\ell_{\phi} \ge N_I$. Indeed, only when the localization length ℓ_{ϕ} , expressed in number of photons, is larger than the number N_I of photons required for ionization, will a non-negligible amount of quantum probability fall into the continuum states, thus leading to ionization.

In order to analyze the ionization process we consider the simple case in which both fields are parallel. Due to the cylindrical symmetry, the magnetic quantum number m is an exact integral of the motion, and the Hamiltonian has the form

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

where $\omega_L = B/c = B(T)/B_0$ is the rotation frequency in a magnetic field, $B_0 = 2.35 \times 10^5 \text{T}$, and ϵ and ω are the field intensity and frequency respectively (atomic units are used).

In the presence of a magnetic field only ($\epsilon = 0$), according to well-known results [8,9], the motion becomes strongly chaotic when $\omega_L n_0^3 \gtrsim 4$ and no islands of stability are observed for $\omega_L n_0^3 \approx 9$. When the microwave field is turned on, diffusive excitation of the electron will take place and the energy diffusion rate D_B per unit time can be estimated in the following way: from Eq. (1), $\dot{E} = -\epsilon z \omega \sin \omega t$ and, therefore, for $\omega_0 \ll 1$ in a quasilinear approximation [10], the diffusion is determined by the spectral density of perturbation. That is, $D_B \sim (\epsilon z \omega)^2 / \delta \omega \sim (\epsilon z \omega)^2 n_0^3 \sim D_0 \omega_0^2$, where $\delta \omega \approx n_0^{-3}$ is a typical frequency at $\epsilon = 0$, and $D_0 = \epsilon^2 n_0/2$ is the diffusion rate in the chaotic regime for B=0 and $\omega_0 = 1$ [11]. Therefore,

$$D_B = \chi_1 D_0 \omega_0^2, \qquad (2)$$

where χ_1 is a constant to be numerically determined. This estimate is a good approximation if $\omega_L n_0^3$ is not too large (the

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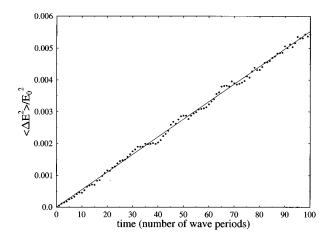


FIG. 1. Example of diffusive energy excitation $\langle \Delta E^2 \rangle / E_0^2$ with time, for parameter values $\omega_L n_0^3 = 9$, $\omega_0 = 0.05$, and $\epsilon_0 = 0.003$. The straight line shows the diffusive growth with a fitted rate given by Eq. (2) with $\chi_1 = 9.8$.

case $\omega_L n_0^3 \ge 10$ should be separately studied). In the regime $\omega_0 \ge 1$, the energy change will take place only when the electron passes close to the nucleus and, in analogy with the case B = 0, the diffusion rate is given approximately by [11] $D_B \simeq \chi_2 \epsilon^2 n_0 \omega_0^{-4/3}/2 = \chi_2 D_0 \omega_0^{-4/3}$. Notice that D_B does not explicitly depend on the magnetic field *B*; however, the quantities χ_1, χ_2 can both weakly depend on *B* for $\omega_L n_0^3 \ge 2$ (see Fig. 3).

In order to check the above analytical estimates for D_B , we have carried out numerical simulations of the classical problem (1). We fixed the magnetic number m=0, and measured the energy excitation for an ensemble of 100 trajectories with the same initial energy $E_0 = -1/(2n_0^2)$. In Fig. 1 we demonstrate the diffusive excitation process in energy for scaled frequency $\omega_0 \ll 1$ and very small microwave field $\epsilon_0 = \epsilon n_0^4$. Here $\omega_L n_0^3 = 9$, so that the motion is fully chaotic even for $\epsilon_0 = 0$.

The frequency dependence of the diffusion rate D_B is shown in Fig. 2 for fixed $\omega_L n_0^3 = 9$. The behavior for small and large frequencies is in agreement with the above theoretical estimates, and is indicated by the two straight lines with $\chi_1 \approx 18$ and $\chi_2 \approx 2$, respectively. An interesting feature is that in a rather large-frequency interval $(10^{-1} \le \omega_0 \le 10)$ the frequency dependence is rather weak. We also checked the ϵ^2 dependence of the diffusion rate D_B by varying the field intensity over a few orders of magnitude.

In Fig. 3 we plot the dependence of D_B on magnetic-field intensity for small values of ω_0 . According to our expectations, the diffusion rate remains approximately constant for $\omega_L n_0^3 > 2$, while below this value the internal motion becomes integrable and diffusion drops to zero.

The classical diffusive process will lead to ionization of the atom after a time $t_I \approx E_0^2 / D_B$. For low-field strength this time is much larger than both the orbital period and the microwave field period, and therefore quantum interference effects can lead to localization of classical diffusion. The localization length ℓ_{ϕ} (in number of photons) can be obtained by using known estimates [12], according to which $\ell_{\phi} \sim \Gamma \rho$, where ρ is the density of coupled states and Γ is the one-photon transition rate, which in turn can be related to

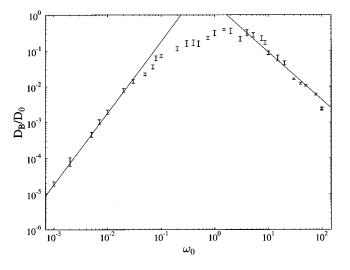


FIG. 2. Dependence of scaled diffusion rate D_B/D_0 on scaled frequency ω_0 for $\omega_L n_0^3 = 9$. Here $D_0 = \epsilon_0^2/2n_0^7$ and ϵ_0 in the interval $10^{-3} \le \epsilon_0 \le 10^{-2}$. The straight lines show the theoretical dependence for $\omega_0 \ge 1$ and $\omega_0 \ge 1$ with $\chi_1 = 18$ and $\chi_2 = 2$, respectively (see text). Ensembles from 30 to 100 orbits have been used.

the classical diffusion rate via $\Gamma = D_B \omega^{-2}$. The striking advantage of such an approach to the computation of the localization length [12] is that it involves only classical characteristics of motion, namely, the classical diffusion rate and density of coupled states. It is therefore sufficient to know only these two quantities to understand the properties of quantum dynamics. In this way one need not worry about quantum matrix elements, the structure of eigenfunctions, and other quantum aspects. This fact becomes even more remarkable if one remembers that without a magnetic field the effective dynamics is well described by a onedimensional atom model [11], while in a strong magnetic field the motion is essentially two dimensional and quite different from the usual Kepler dynamics.

For zero magnetic field the effective density of coupled states is $\rho = n^3$, due to Coulomb degeneracy and the exist-

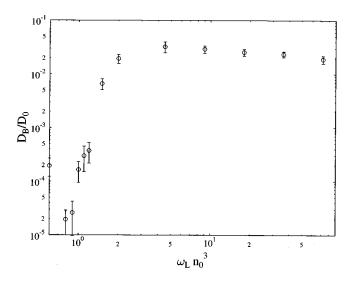


FIG. 3. Scaled diffusion rate D_B/D_0 as a function of the scaled frequency $\omega_L n_0^3$ for $\omega_0 = 0.05$ and $\epsilon_0 = 0.003$.

ence of an additional approximate integral of motion [11]. Instead, for sufficiently large *B*, the internal motion is chaotic and the density of coupled states is $\rho = n^4$. Therefore, in the latter case the localization length in number of photons is

$$\ell_{B} = \ell_{\phi} \frac{D_{B}}{D_{0}} \frac{n_{0}}{\omega_{0}^{2}}, \tag{3}$$

where $\ell_{\phi} = 3.3\epsilon_0^2 n_0^2$ is the localization length in the microwave field only (B=0) at $\omega_0 = 1$ and it is assumed that $l_B > 1$.

For $\omega_0 \ll 1$ we obtain $\ell_B = 3.3\chi_1 \epsilon_0^2 n_0^3$ from Eq. (3). The delocalization border, namely, the critical microwave field intensity ϵ_1 above which ionization takes place, is given by the condition $\ell_B = N_I$, leading to

$$\boldsymbol{\epsilon}_{01} = \frac{1}{n_0 \sqrt{6.6 \chi_1 \omega_0}} \tag{4}$$

which is well below the delocalization border within the microwave field alone. We would like to stress that the above estimates are valid in the regime $\omega \rho > 1$ [12], that is, $\omega_0 > n_0^{-1}$ [and therefore the border Eq. (4) is valid for $n_0^{-1} < \omega_0 < 1$].

The above estimates were made in analogy to the problem of photonic localization in a random molecular quasicontinuum [12]. However, it is possible that such an approach should be modified for the present case of a well-defined quasiclassical system with adiabatically slow perturbation. Indeed, in such a situation, one can make a transformation to an instantaneous time basis in which transition matrix elements are proportional to the frequency of the perturbation. Here, many levels will be mixed only if this effective matrix element $V_{\rm eff}$ proportional to ω is larger than the level spacing in one atomic shell n^{-4} . For a chaotic case we can estimate $V_{\rm eff} \sim \epsilon \omega n^5 / \sqrt{n}$, so that the diffusive exitation is quasiclassical (nonperturbative) only if $V_{\rm eff} > 1/n^4$. The same estimate can be also understood in the following quasiclassical way. The diffusion rate in the number of shells (the change of the principal quantum number in the unperturbed hydrogen $\Delta n = 1$) is $D_n = D_B n^6$. All the levels in the shell will be resolved after time $t_{\rm sh} \approx 2 \pi n^4$. Therefore, the adiabatic perturbation is perturbative if the number of shells mixed during this time is less than 1: $(\Delta n)^2 \approx D_n t_{\rm sh} < 1$. The situation is quasiclassical in the opposite case $(\Delta n)^2 > 1$ when

$$\boldsymbol{\epsilon}_0 > \boldsymbol{\epsilon}_{0a} \approx \left(\frac{1}{3\chi_1}\right)^{1/2} \frac{1}{\omega_0 n_0^{3/2}}.$$
 (5)

In this regime the diffusion rate measured in the number of shells per unit of time τ measured in units of $t_{\rm sh}$ is $D_{\rm sh} = (\Delta n)^2 / \Delta \tau \approx 3 \chi_1 \epsilon_0^2 \omega_0^2 n_0^3 > 1$. Similarly to the standard estimate [12] this diffusion will be localized after time $\tau^* \approx D_{\rm sh}$ with localization length $l_n \approx \Delta n(\tau^*) \approx D_{\rm sh}$ (in the number of photons this gives $l_B = l_n / \omega_0 = D_{\rm sh} / \omega_0$). Then the delocalization border is determined by the condition $l_n \sim n_0/2$, giving

$$\epsilon_0 > \epsilon_{0qa} \approx \frac{1}{\sqrt{6\chi_1}\omega_0 n_0}.$$
 (6)

As we see, these adiabatic estimates are different from the above Eqs. (3) and (4). In our opinion the physical situation is more correctly described by the approach (3) and (4). However, only direct quantum simulations or laboratory experiments can lead to more definite conclusions.

For $\omega_0 \ge 1$ the situation is more standard, and we have

$$\ell_B = 3.3 \chi_2 \frac{\epsilon^2}{\omega^{10/3}} n_0, \tag{7}$$

and the condition $\ell_B = N_I$ leads to

$$\epsilon_{02} = \frac{\omega_0^{7/6}}{n_0 \sqrt{6.6\chi_2}},\tag{8}$$

which is $\sqrt{n_0\chi_2}$ times smaller than the quantum delocalization border for B=0.

It is important to remark that, contrary to the case B=0, the localization length depends now on photon number. Indeed, for $\omega_0 \ll 1$, $\ell_B \propto n_0^{11} \sim (N_I - N)^{-11/2}$ while for $\omega_0 > 1$, $\ell_B \propto n_0 \sim (N_I - N)^{-1/2}$. This means that localization length becomes larger near the ionization border. However, this effect is not important if $\ell_B \ll N_I$ while for $\ell_B \approx N_I$ it will lead to a change in the numerical factor for the delocalization border. We also remark that for $\omega_0 \ll 1$ the quantum delocalization border ϵ_{01} will be relevant only if it remains smaller than the ionization border for a static electric field in the presence of a parallel magnetic field.

Finally, we would like to stress that, to our knowledge, the problem under investigation represents a qualitatively new situation as compared to the hydrogen atom in a microwave field only. Therefore, the above preliminary estimates require a detailed check by quantum simulations.

On qualitative grounds, the effects described in the present paper can also take place in nonhydrogen atoms in a static electric field and in the absence of a magnetic field. It is indeed known that, for nonhydrogen atoms in static electric fields, the eigenfunctions can be approximately ergodic, and the level spacing statistics shows a level repulsion of the Wigner-Dyson type [13]. This situation is similar to that in which internal chaos is present due to a strong magnetic field. Since in the formulas derived in this paper the magnetic-field dependence is quite weak, we expect that they are approximately valid even for nonhydrogen atoms in static electric fields. However, one should keep in mind that while qualitatively the ionization process should behave similarly to the case with a magnetic field, the chaos properties in a static electric field are not so strong, and therefore this case should be analyzed in more detail. Such a situation with atoms in a static electric field is quite interesting since it is more suitable for laboratory experiments. Finally, we believe that the results described in the present paper will not be significantly changed if the electric and magnetic fields are not parallel, provided that the electric field is relatively weak. The reason for this is that the magnetic quantum number m will determine the existence of an approximate integral of motion similar to the case of hydrogen in a microwave field [11].

In this paper we have introduced and discussed a model that should allow for a clear experimental investigation of quantum-dynamical localization. Its main feature is the wide range inside which it is possible to change physical parameters such as ω_0 , ϵ_0 and the interaction time. A possible convenient choice of parameters is $n_0=60$, $\omega_0=0.1$ ($\omega=3.0$ GHz), and B=10 T ($\omega_L n_0^3=9$) (or static electric field $\epsilon_{0st}\approx 0.05$ for nonhydrogen atoms). For these conditions we have $\epsilon_{01}=0.005$, $N_I=300$, and interaction time (mea-

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sured in number of microwave periods) $\tau_I = \omega t_I/2 \pi = (1/4\pi\chi_1)/(\epsilon_0^2\omega_0) \approx 1800$. If, however, we define the ionization probability as the occupation probability of levels n > 70, then the number of photons will be $N_I \sim 100$ and the ionization time $\tau_I = 180$ microwave periods. This range of parameters seems to be suitable for laboratory experiments.

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