Localization of Diffusive Excitation in the Two-Dimensional Hydrogen Atom in a Monochromatic Field

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We present new data from numerical simulations of microwave excitation of a two-dimensional hydrogen atom, which show that in a wide parameter range under the one-dimensional delocalization border, the quantum localization phenomenon persists. We theoretically reconsider the problem of two-dimensional localization, by using an appropriately constructed four-dimensional map over an orbital period of the electron, and thus explain the numerical results.

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We recently reported[1-3] about our extensive studies of a one-dimensional model for a highly excited hydrogen atom in a linearly polarized monochromatic microwave field. The most interesting effect which was numerically observed and theoretically explained was the localization of the diffusive excitation under the condition

$$\epsilon_0 < \epsilon_q^{(1)} \approx \omega_0^{7/6}/(6n_0)^{1/2}. \qquad (1)$$

Here, $n_0 \gg 1$ is the initially excited level, $\epsilon_0 = \epsilon n_0^4$ and $\omega_0 = \omega n_0^3$ are the rescaled field strength and frequency, and all physical variables are in atomic units. We also checked the validity of the one-dimensional model for extended states (with parabolic quantum number $n_2 = 1$ and magnetic quantum number $m = 0$) by means of a two-dimensional model [see Fig. 7(c) of Ref. 3], which made use of a basis of unperturbed bound-state eigenfunctions, up to $n = 128$. A theoretical explanation was also given[1,3] together with a rough estimate for the two-dimensional delocalization border:

$$\epsilon_q^{(2)} \sim \omega_0^{7/6}(n_2 n_0)^{1/2}. \qquad (2)$$

Here we report about preliminary results of two-dimensional numerical simulations with initial conditions $n_0 = 66$, $n_2 \leq 30$ (which is about the largest possible value) and parameter values $0.04 \leq \epsilon \leq 0.06$ and $\omega_0 = 1.5$ and 2.5. Since two-dimensional computations are much more time consuming, we had to restrict our simulation to a relatively short number of field periods, $\tau \leq 120$. In Fig. 1(b) we show a typical two-dimensional behavior, for both the quantum and the corresponding classical models. From Figs. 1(a) and 1(b) it is apparent that the quantum motion in the principal quantum number n is localized. This is also confirmed by Fig. 2, where

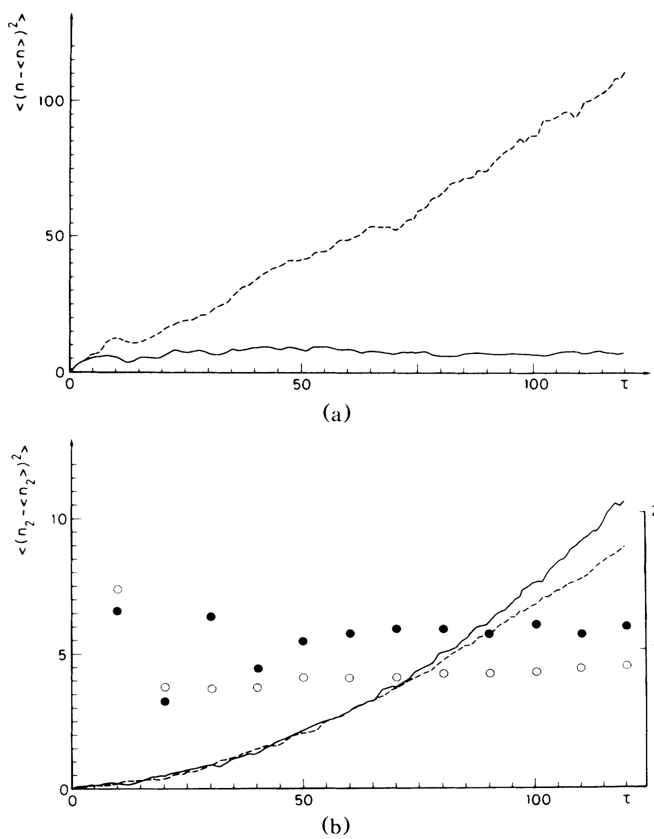

FIG. 1. Classical (dashed curve) and quantum (full curve) numerical results for the two-dimensional hydrogen atom under a microwave field. Here $n_0 = 66$, $\omega_0 = 2.5$, $\epsilon_0 = 0.04$, $n_{20} = 15$, and τ is time measured in number of field periods. (a) Second moment μ_2 of n. (b) Second moment μ_2 of n_2. We also show the ratio of μ_2/n_{20} to the first moment μ_1 of n_2 in the classical case (open circles) and in the quantum case (full circles). It is seen that this ratio is close to 1 (right-hand scale).

the classical and quantum distributions integrated over n_2 are plotted versus the number of absorbed photons (which, as shown in Ref. 4, more conveniently exposes the localization phenomenon). Moreover, in all the investigated cases, the localization length is satisfactorily described by the one-dimensional estimate.[1,3,4]

Two relevant facts emerge from these data: (i) Fig. 2 shows that the n motion remains essentially one-dimensional independently of the value of n_2; (ii) the n_2 motion has a qualitatively different character, namely, it shows no localization (in the sense that the quantum n_2 motion remains close to the classical one at least in the inspected time interval) [Fig. 1(b)]; yet this fact has no impact on the localization occurring for the n motion (Fig. 2). Thus the picture emerging from numerical results is completely different from the one assumed in deriving the estimate (2).

In the attempt at understanding the above numerical results, we developed a new theoretical approach, which is a two-dimensional generalization of the theory of Ref. 4. The two-dimensional Hamiltonian in action-angle variables is[5,6]

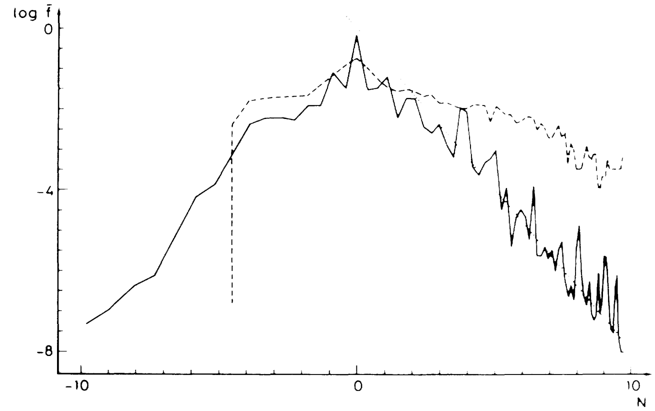

FIG. 2. Classical (dashed curve) and quantum (full curve) distribution functions, averaged in the time interval $110 < \tau \leq 120$, vs the number of absorbed photons $N = [(2n_0^2)^{-1} - (2n^2)^{-1}]/\omega$ (Ref. 4) for the same parameter values as in Fig. 1. The straight line is the one-dimensional theoretical exponential distribution.

$$H = -\frac{1}{2n^2} + \epsilon n^2 \cos\omega t \left[\tfrac{3}{2} e \cos\psi - 2 \sum_{s=1}^{\infty} (x_s \cos s\theta \cos\psi - y_s \sin s\theta \sin\psi) \right].$$

e is the eccentricity $[e = (1 - l^2/n^2)^{1/2}$ with l the orbital momentum], and the Fourier amplitudes x_s, y_s are

$$x_s = s^{-1} J_s'(es), \quad y_s = (se)^{-1}(1-e^2)^{1/2} J_s(se).$$

θ is the azimuthal angle, ψ is the angle conjugate to l, i.e., it is the angle between the major axis of the ellipse and the direction of the field. Under the assumptions

$$\omega n^3 \gg 1, \quad l/n < (2/\omega_0)^{1/3}, \tag{3}$$

x_s, y_s admit the asymptotic expansions

$$x_s \approx (0.411/s^{5/3})(1 + l^2/2n^2),$$

$$y_s \approx (l/n) 0.447/s^{4/3}.$$

If (3) are satisfied, then $l \ll n$ and e is close to 1. Actually, the error involved by these asymptotical expressions even for $\omega n^3 \simeq 1$ is only $\simeq 30\%$. We derived a convenient approximate description of the 2D dynamics by means of a 4D map. This map describes the change, during one orbital period of the electron, of the canonical variables N, l, ϕ, ψ, where N is energy divided by ω $(N = -1/2n^2\omega)$, and ϕ is the phase canonically conjugate to N (ϕ is just the product of ω by the time and Ψ is the angle between the major axis of the ellipse and the external field). We found this map by integrating the exact Hamiltonian equations of motion over one orbital period; while doing so, we substituted the unperturbed motion in the field-dependent terms and we kept only the resonant term of the perturbation.

As a result, we found that the generating function of the map leading to the new values $(\bar{N}, \bar{l}, \bar{\phi}, \bar{\Psi})$ is

$$G(\bar{N}, \phi, \bar{l}, \Psi) = \bar{N}\phi + \bar{l}\Psi - 2\pi(-2\omega\bar{N})^{-1/2} - k[(1 - \omega\bar{N}\bar{l}^2)\cos\phi\cos\psi - 1.09\omega^{1/3}\bar{l}\sin\phi\sin\psi], \tag{4}$$

where $k = 2\pi \times 0.411\epsilon/\omega^{5/3}$. The details of the derivation of Eq. (4) will be presented elsewhere.[7]

In deriving (4), we assumed conditions (3) which ensure that the Fourier components of the perturbation decay according to a power law. In order to simplify the map, it is convenient to go over to new canonical variables (N, J, θ, χ) (Refs. 5 and 6) defined by

$$\tan\chi = (B/A)\tan\psi, \quad \theta = \phi + \chi,$$
$$J + N = \int_0 dl' AB/(A^2 \sin^2\chi + B^2\cos^2\chi), \tag{5}$$
$$A = 1 - N\omega l^2, \quad B = 1.09\omega^{1/3} l.$$

In these new variables the map is given by

$$\begin{aligned} \bar{\chi} &= \chi - k(\partial H/\partial \bar{J})\cos\theta, \\ \bar{J} &= J + k(\partial H/\partial \chi)\cos\theta, \\ \bar{N} &= N - kH\sin\theta, \\ \bar{\theta} &= \theta - 2\pi\omega(-2\omega\bar{N})^{-3/2} - k(\partial H/\partial \bar{N})\cos\theta, \end{aligned} \tag{6}$$

where $H^2(\bar{J}, \bar{N}, \chi) = A^2\cos^2\psi + B^2\sin^2\psi$.

A decisive simplification of the dynamics described by (6) would be gained under a couple of assumptions that would allow for a sort of decoupling of the (N,θ) from the (J,χ) dynamics. These conditions are (i) that the change in J and χ in one step be small, so that a continuous-time approximation for the first couple of Eqs. (6) is valid, and (ii) that H be only weakly dependent on N. Conditions for (i) and (ii) will be specified below. With the assumption (i), the (J,χ) equations become

$$\dot{J}=k\cos\theta\,\partial H/\partial\chi,\quad \dot{\chi}=-k\cos\theta\,\partial H/\partial J,$$

and if we introduce a new time σ by $d\sigma/dt=k\cos\theta$ (t is the number of iterations) the (J,χ) dynamics is ruled by the Hamiltonian H, which is therefore a constant of the (J,χ) motion; in other words H can change in time only through changes in N. Then, with use of (ii), the (N,θ) equations become almost identical to the 2D mapping described in Ref. 4 and the (N,θ) motion is strictly one dimensional. For approximately one-dimensional states ($l\ll n$, $\psi\ll 1$), $H\approx 1$ and the (N,θ) equations coincide with the one-dimensional equations[4]; moreover, in the new time σ, the motion in the (χ,J) variables will not depend on the (N,θ) motion.

However, since the connection of the time σ with the real time t is defined by the (N,θ) dynamics, the real-time (χ,J) dynamics has a different character according to whether the (N,θ) motion is regular or chaotic.

To see this we first consider a case in which a regular motion in (N,θ) is taking place with $\lambda=\langle\cos\theta\rangle\neq 0$. (This may happen also above the chaotic threshold, because of the presence of stable regions.[3]) Then $\sigma\approx k\lambda t$. For nearly one-dimensional states and $\psi\ll 1$, the Hamiltonian H can be approximately written as

$$H=1+\tfrac{1}{2}(l^2/n^2-\psi^2), \tag{7}$$

with n constant. The (l,ψ) motion described by (7) is unstable, with a characteristic instability time $\sigma_{\bar{l}}=n$ or $t_{\bar{l}}=n/k\lambda$, as was pointed out in Ref. 6. [Nevertheless, the long-term motion is certainly periodic, with a period $T_{\bar{l}}\sim 2t_{\bar{l}}\Lambda$, where $\Lambda\sim\ln(n/n_2)$.] Thus one condition for the continuous-time approximation (i) to hold is $t_{\bar{l}}\approx\omega_0^{5/3}/(2.6\epsilon_0\lambda)\gg 1$.

In the opposite case of completely chaotic (N,θ) motion, $\sigma(t)$ is a random function with $\langle\sigma(t)\rangle=0$, $\langle\sigma^2(t)\rangle=k^2t/2$. Then the average of the exponent σ/n in the solution of (7) is given by $\langle(\sigma/n)^2\rangle=k^2t/(2n^2)$, whence we see that the characteristic time of the motion is now $t_{\text{ch}}=2(n/k)^2\gg t_{\bar{l}}$. This time can be compared with the ionization time $t_I\approx 2N_0^2/k^2$, with $N_0=-1/2n_0^2\omega$, with the result that $t_{\text{ch}}/t_I\approx 4\omega_0^2\gg 1$. Therefore the chaotic precession is completely unimportant for the N motion. Notice that the (χ,J) motion can be depicted as a random walk taking place along an invariant curve $H=$const.

If the Hamiltonian (7) is written in the variables N,ψ ($N=-1/2n^2\omega$), the approximate equation $\delta H\sim\omega l^2\delta N$ is obtained, and a condition under which the N dependence of H can be neglected takes the form $\omega l^2\delta N<l^2/n_0^2\ll 1$. Even though the latter condition is formally necessary for the above theory to hold, the strong inequality $l^2/n_0^2\ll 1$ is not crucial. Indeed our numerical results (Figs. 1 and 2) indicate that, even when $l\sim n$, the main qualitative result of our analysis remains valid, i.e., the slow precession taking place in the n_2 motion does not affect the n motion, which remains approximately one dimensional. For this reason the 1D estimates still hold, except when H assumes values $\ll 1$. Details will be given in a forthcoming paper.[7] Then, turning to the quantum case, we get the usual one-dimensional localization for the N motion, with the localization length $L\approx(k^2/2)H^2\approx k^2/2$, independently of the (l,ψ) dynamics. This explains the behavior observed in our numerical computations (Figs. 1 and 2).

On the other hand, the n_2 motion exhibits a regular quadratic increase in spite of the classical chaotic (N,θ) motion. This can be explained by the above theory. Indeed, using the explicit solution for the motion described by (7), and using the relation $(n_1-n_2)/n=(1-l^2/n^2)^{1/2}\cos\psi$ which approximately gives $n_2\approx\frac{1}{4}(l^2/n+n\psi^2)$, we get

$$n_2\approx n_{20}[\cosh(2\sigma/n)+(\sin 2\eta_0)\sinh(2\sigma/n)], \tag{8}$$

where η_0 is the initial value of the phase conjugate to n_2, that must be assumed to be uniformly distributed in $(0,2\pi)$ in order to reproduce the initial quantum state. From (8), by phase averaging, we find the dependence of the first two moments of n_2 on the time σ:

$$\begin{aligned}\mu_2&=\langle(n_2-\langle n_2\rangle)^2\rangle=(n_{20}^2/2)\sinh^2(2\sigma/n);\\ \mu_1&=\langle n_2-n_{20}\rangle=n_{20}[\cosh(2\sigma/n)-1].\end{aligned} \tag{9}$$

For $2\sigma/n\ll 1$, the ratio $\mu_2/\mu_1\approx n_{20}$, which reasonably agrees with numerical data [Fig. 1(b)]. From the comparison of (9) with numerical data we can calculate the regular characteristic time: $\tau_{\bar{l}}\approx 750$. Then we can also find the corresponding values of the factor λ which relates the times τ and σ: $\lambda\approx 0.14$. The fact that λ is nonzero is due to the presence of stable regions in the (N,θ) motion. On the other hand, its relatively small value may be related to the fact that the frequency $\omega_0=2.5$ lies just between two main resonances, so that the stable region is small for the chosen initial conditions. Then the instability in the n_2 motion is a very slow one.[3]

The next important question is what the impact of a change in H on the (N,θ) dynamics would be, and whether, in particular, it could lead to two-dimensional delocalization. In our opinion this could not happen, unless t_{ch} becomes comparable with the localization time $\sim L$. Indeed, the (l,ψ) motion would just broaden the lines in the discrete spectrum of the (N,θ) motion, up to a width $\sim 1/t_{\text{ch}}$. In order to provide delocalization, it is at least necessary (but perhaps not yet sufficient) that $t_{\text{ch}}^{-1}>L^{-1}$ (the average spacing in the discrete spectrum) or $L > t_{ch}$. This cannot happen below the one-dimensional delocalization border, because the ratio $t_{ch}/L \sim (\epsilon_q^{(1)}/\epsilon_0)^4 \omega_0^2 > 1$. In other words, the slow (l,ψ) motion acts as an adiabatic perturbation on the (N,θ) motion, and cannot produce any additional transition in the latter. The ultimate reason for this adiabaticity is Coulomb degeneracy.

Therefore it appears that in order for any truly two-dimensional delocalization to occur, the approximate conservation of H must be destroyed, and a sufficiently short time scale for the (l,ψ) motion must be provided. Our previous estimate (2) failed because, in deriving it, both these conditions were implicitly assumed. We conjecture, and are currently investigating, that both these conditions can be satisfied by introduction of a relatively strong static field.[8] Without static field the localization of diffusive excitation appears to be as typical a phenomenon in the two-dimensional case as it was found to be in the 1D one.

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[8]This would contradict the stabilizing effect of a strong static field predicted in Ref. 6 since the stabilized precession may be nevertheless chaotic. A discussion of this problem is given in Ref. 7.