Classical aspects of quantum localization in microwave ionization of H atoms

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It is shown that the main part of the differences between classical and quantum predictions concerning the microwave ionization of H-atom threshold frequency dependence, commonly explained as a manifestation of quantum localization, originates from the enhanced, in classical simulations, role of the Coulomb singularity. When the Coulomb potential is softened, classical simulations reproduce quantum predictions and experimental data satisfactorily. No interference, intrinsically important for localization phenomena, is necessary.

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The studies of microwave ionization from initial Rydberg states of the H atom commenced more than twenty years ago [1]. The experimental data (for microwave frequencies \(\omega < \omega_K\), the Kepler frequency of initial state) could be reproduced by classical simulations [2] suggesting chaotic classical diffusion as a mechanism of the ionization. However, it was shown that for the so called kicked rotator model, quantum behavior at high frequencies exhibits a localization phenomenon which, for that particular model, may be mapped into the known Anderson solid-state problem [3]; thus the localization in the kicked rotator is equivalent to Anderson localization in disordered solids. Since the kicked rotator (and the corresponding classically standard map) should be a good local approximation to dynamics for a generic system [4], it has been postulated (and supported by approximate quantum results) that for high frequencies, i.e., \(\omega > \omega_K\) or \(\omega_0 > 1\) (where \(\omega_0 = \omega/\omega_K\) is the scaled frequency) the discrepancy should appear between classical predictions and experimental (or quantum) ionization threshold values. A number of theoretical studies has supported this picture (we refer the reader to [5,6] for an extensive list of references; the most complete quantum study of the problem will appear in [7]). Importantly it was also found experimentally [8,9] (see also reviews [10,11]) that the microwave amplitude needed to produce a 10\% ionization (a commonly accepted value for the threshold) was significantly higher than the classical simulation values. Since then, it has been commonly accepted that this difference in threshold values is indeed a manifestation of a quantum localization phenomenon in microwave ionization experimentation. A further step toward forming a localization picture has been the realization that at high frequencies the main mechanism of excitation is due to collisions of the electrons with the nucleus. This made it possible to convert the continuous dynamics (in the monochromatic microwave field) into the discrete-time evolution—the so called Kepler map [6], bringing the analogy to kicked rotators even closer.

Still, the connection between the classical-quantum disagreement for high frequency microwave ionization thresholds and the quantum localization theory (in Anderson sense) is quite indirect, and no rigorous argument similar to that presented for the kicked rotator [3] exists. One may imagine a different explanation for these differences. In particular, MacKay and Meiss [12] have shown that the classical slowdown of the diffusion due to the remnants of regularities in the phase space, the so called cantori, may be greatly enhanced in the quantum world due to the coarse graining of the phase space (and gluing of “holes” allowing for diffusion) introduced by a finite value of \(\hbar\). This theory reproduced the experimental data quite well [13].

The aim of this paper is to reexamine the problem using classical simulations only but, at the same time, taking into account in some way the effects due to finite \(\hbar\) values. Within the classical mechanics, the only possible way to do this is to modify (in a physically acceptable way) the Hamiltonian of the problem, which reads (in atomic units)

\[
H = \frac{p^2}{2} - \frac{1}{r} + zF(t) \sin(\omega t + \phi),
\]

where \(F(t)\) and \(\phi\) are the envelope and the initial phase, respectively, of the microwave pulse polarized along the Oz axis. Its prominent feature is a Coulomb singularity, the most important feature for high frequencies, since, as mentioned above, close electron-proton encounters facilitate excitation in the atom. Naturally, quantum mechanics smooths the singularity due to the Heisenberg uncertainty principle. That was pointed out by Leopold and Richards [14], who found the condition for the breakdown of classical mechanics description within a pure Coulomb model. As mentioned above, we wish to stay within classical mechanics but modify the potential. Smoothing in the immediate vicinity of the nucleus would be a suitable modification. Such an approach has already been successfully used in simulating classically the quantum mechanics for the phenomenon of adiabatic stabilization for ionization from low lying states by the superstrong laser field [15,16]. Here we propose to use the same approach for the present problem. The modified potential takes the form

\[
V(r) = 1/\sqrt{r^2 + a^2},
\]

where \(a\) is a constant, the value of which should be physically motivated or fitted to the data.

A further simplification is possible. Most of the theoretical quantum results for the microwave ionization problem
have been obtained using the simplified one-dimensional model of the atom. The model is well justified—in experiments [10,11], initial states of a given principal quantum number \( n_0 \) are selected but no selection of other quantum numbers is made. Thus atoms enter the microwave region in a mixture of different angular-momentum states. The thresholds are then determined by the field values leading to ionization of most vulnerable states. For linearly polarized radiation, those are states elongated along the polarization direction for which a one-dimensional atomic model is reasonable. Of course, we may perform the same simplification for our smoothed Coulomb problem; moreover, this approach actually gains physical significance in this way.

Note that the original Coulomb potential may be written as \( V(r) = 1/\sqrt{r^2 + \rho^2} \), where \( \rho \) is the distance to the nucleus in the plane perpendicular to the polarization axis. Indeed, for the elongated states, the range of relevant motion along the \( O_3 \) axis exceeds that in the perpendicular direction (eventually leading to ionization preferentially along the \( z \) axis). Thus one may make an adiabatic approximation and consider the motion along the \( O_3 \) axis only in the averaged potential \( \overline{V(r)} = 1/\sqrt{\langle r^2 \rangle + \langle \rho^2 \rangle} \), where the averaged \( \rho \) now appears in the denominator. Thus we may restrict the dynamics to the one-dimensional model:

\[
H = \frac{P^2}{2} - \frac{1}{\sqrt{\omega^2 + a^2}} + zF(t) \sin(\omega t + \varphi),
\]

where constant \( a \) may now be directly related to \( \sqrt{\langle \rho^2 \rangle} \) (\( P \) denotes the momentum conjugate to \( z \)). Note that the Hamiltonian (3) has been extensively used in the study of ionization by superstrong laser pulses [17].

The latter allows us to set the "limits of common sense" on the possible values of \( a \). Consider the scaled problem as it is commonly done [5,6,10], i.e., instead of looking at evolution for a given initial principal quantum number, \( n_0 \), corresponding to classical energy \( E = -(1/2)a^2 \) for some \( F \) and \( \omega \) values, we use the classical scaling and consider the equivalent evolution for \( E = -1/2 \) and scaled frequency \( \omega_0 = n_0 \omega = a/\omega \) (introduced previously) and the scaled microwave amplitude \( F_0 = n_0 F \). Since the extension of the ground state in atomic units is of the order of unity, \( a \) should be chosen between 0 and 1.

Having set the stage, let us now present the details of the numerical simulations performed using the Hamiltonian Eq. (3), and a comparison with both the experimental results and the quantum localization theory predictions. The classical simulations has been performed in a way allowing for a comparison with the experimental data presented in [10]. The microwave pulse envelope has been chosen in accordance with the experimental pulse in the TM \(_{00}\) mode. In that experiment, the excitation above some threshold energy value, corresponding to maximal principal quantum number \( n_C \), rather than the true ionization, is measured. The cutoff \( n \) value, \( n_C \), varies from one set of data to the other—we change the classical energy cutoff accordingly. The actual numerical integration of equations of motion is carried out in scaled variables, with the appropriately rescaled cutoff energy. The sample of initial conditions is chosen uniformly and randomly on the initial torus of the unperturbed modified Coulomb problem for a given \( a \). Since no explicit form for the action-angle variables is available for \( a > 0 \), we first determine the period of the motion, \( T_p \), then choose uniformly and randomly a set of times \( t_i \in [0,T_p] \), \( i = 1, \ldots, N \), where \( N \) is the size of the sample. Starting from a turning point and integrating the unperturbed motion up to \( t_i \) gives us the initial conditions \( z_i, p_i \) for the \( i \)th trajectory. The trajectories contribute to "effective" ionization if their final energy, after the pulse has died out, is greater than the appropriate cutoff energy. An additional average is performed over the initial phase of the microwave pulse \( \varphi \). Varying the maximal pulse amplitude, we determine the values of \( \varepsilon_0 \), the amplitude at which a 10% effective ionization is obtained.

In the experiment, not the frequency but rather the initial \( n_0 \) is varied. We perform the simulation in an analogous way, keeping for all \( n_0 \) the same value of the scaled smoothing parameter, \( a \) [18]. The results of numerical simulations for two sets of experimental data are presented in Figs. 1 and 2. Comparison of two simulations with values of \( a = 0.4 \) and \( a = 0.5 \) is presented in Fig. 1 together with the experimental data and the prediction of the localization theory based on the formula [19]

\[
\varepsilon_0 = \frac{\omega_0^{\text{c}}}{{\sqrt{8}} \sqrt{1 - \frac{n_C^2}{n_0^2}}} \omega_0,
\]

which also takes into account the effective threshold. Note that the simulation for \( a = 0.4 \) reproduces the average trend in the experimental data quite well, while \( a = 0.5 \) better approximates the results of the localization theory. By comparison, the simulations for the pure one-dimensional Coulomb problem, equivalent to the so-called classical chaos border [5], fall well below and decrease with increasing \( \omega_0 \). Also, the classical three-dimensional simulations [20] significantly underestimate the threshold.

The constant \( a \) should vary little from one data set to the other. Figure 2 presents a comparison for the same value
FIG. 2. Comparison of localization theory prediction and $a=0.5$ classical simulation for higher cutoff, $n_C=114$. Same notation as in Fig. 1.

$a=0.5$ and quite different $n_C$. Again, the agreement with the predictions of the localization theory, Eq. (4), is of the same quality as that presented in Fig. 1.

Localization theory predicts, however, not only the threshold values but actually the full distribution over the final $n$ states reached. The distribution shows a characteristic maximum around $n=n_0$, as discussed, e.g., in [14]. We present in Fig. 3 distributions obtained for two values of the field, one well below the threshold, the other above it. While a detailed comparison with calculated quantal distributions would be necessary to draw definite conclusions, the distributions presented in Fig. 3 resemble quantum predictions [15,21] as well as experimental results [22]. Note that for lower microwave amplitude values, the distribution is strongly concentrated around the initial $n_0$, although the value chosen is above the classical chaos border for the pure Coulomb potential. The distribution broadens for $F=0.15$ but shows "localized character" (note the logarithmic vertical scale).

To conclude, we have shown that smoothing of the Coulomb singularity, previously used in classical studies of sta-

FIG. 3. Distribution of final $n$ values obtained for $a=0.5$ classical simulations. Since the classical distribution of final energy $n$ values is continuous, points correspond to the bins in the appropriate histogram. The data correspond to $n_0=72$ (for $\omega=36.02$ GHz, i.e., $\omega_0=2.043$), $n_C=114$, and two amplitudes $F_0=0.03$—circles (above classical chaos border for Coulomb potential but well below the 15% threshold value $\epsilon_0=0.069$), and $F_0=0.15$—triangles (above the 15% threshold).

bilization in strong laser fields [15,16], has allowed us to recover quantum (or experimental) average ionization threshold behavior in the regime of high frequencies. The same physically motivated smoothing also yields, in effect, reasonable final-state distributions, similar to that obtained using full quantum numerical or experimental results. Our results indicate that the present experimental data provide no real evidence of quantum localization (of the Anderson type). After all, while smoothing of the Coulomb singularity to some extent includes effects due to the finite value of $\hbar$, no interference, inherent in full quantum treatment, and intrinsically important in Anderson localization phenomena, is present in our classical simulations.

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[18] Note that the $a = 0.5$ value used is scaled to ground-state energy. In standard units, since length scales as $n_0^2$ for the state with principal number $n_0$, the corresponding $a$ should be multiplied by $n_0^2$. Interpretation in terms of $(\rho^2)$ suggests that elongated states with $l < n_0/2$ contribute to the threshold determination.


