Ionization of the surface-state electron by half-cycle electric-field pulses

T. F. Jiang
Institute of Physics, National Chiao Tung University, 1001 Ta-Hsueh Road, Hsinchu 30050, Taiwan
(Received 13 August 1996)

The purpose of this research is to study the half-cycle pulse (HCP) ionization behavior of the surface-state electron (SSE). Motivated by the experimental progress in the HCP source, we propose to investigate the HCP excitation of the SSE system, which was confirmed to be one dimensional in nature. We examine the cases with a wide range of scaled electric-field amplitudes, which have different time scales and pulse shapes. Our results show some stabilization windows for the ionization probability with respect to these fields. The number of windows increases with the length of the pulse duration. The origin of the window is shown to be related to the energy gained from the driving electric fields. [S0163-1829(97)03808-3]

I. INTRODUCTION

Recently, Jones, You, and Bucksbaum measured the ionization probability of sodium Rydberg states with respect to the field amplitude for a subpicosecond half-cycle pulse (HCP).[1] They also measured the ionization probability of Stark states under HCP.[2] The HCP used is a short electromagnetic pulse with unipolarity. The pulse duration is of the time scale as the Kepler period of the Rydberg states. Instead of some hundreds of driving cycles in a typical pulsed laser-atom ionization experiment, in the HCP experiments the field is turned off within a single Kepler period. These experiments are explorations in atomic excitation and attract a lot of theoretical interest.[3]

In this paper, we address the ionization dynamics of the surface-state electron (SSE) under HCP, rather than the atomic Rydberg states, for the one-dimensional property of SSE discussed below. The electron on a liquid helium surface is attracted by its own image charge, and the Pauli exclusion keeps the surface electron from the helium nuclei. The binding energy of SSE is meV, while the repulsive barrier is of the order of eV. So the electron Hamiltonian for the SSE under external field E is modeled as[4]

$$\hat{H}=\frac{\widehat{p^2}}{2}+\begin{cases}-Z/z\pm zE & \text{if } z>0\\ \infty & \text{if } z\leqslant 0,\end{cases} \tag{1}$$

where $Z=(\epsilon-1)/4(\epsilon+1)$ and $\epsilon=1.057\,23$.[4] The hydrogenic model gives correct experimental bound level transition frequencies up to high excited states.[4] With the parameter, the transition frequency between $n=2$ and $n=1$ is 0.12 THz and the nuclear field strength for the ground state is 1.73 kV/cm, which are in the range of the experimentally feasible HCP region. With this Hamiltonian, Jensen studied the microwave ionization of the excited SSE and explored the classical manifestations of quantum chaos.[5] It also has been widely used, as in the study of microwave ionization of a Rydberg atom,[6] in atomic strong field ionization,[7] in Coulomb scattering problem,[8] and in multiphoton dynamics of Rydberg wave packet in microwave fields.[9] However, the HCP ionization of SSE has not been studied yet to our knowledge, either experimentally or theoretically. Since it is a physically one-dimensional system, the study of its ionization behavior under the new electromagnetic source would be interesting.

First, we will briefly describe our method of calculation, and then present our results. The length unit used is the effective bohr, $a_0=a_b/Z$, energy unit is $E_0=-13.6\ Z^2$ eV, the frequency unit is $\omega_0=4.1341\times10^{16}\ Z^2\ \text{sec}^{-1}$, and the electric field unit is $F_0=5.142\times10^9\ Z^3$ V/cm, where $a_b=0.5292$ Å. For the excited state n, the corresponding frequency is $\omega_n=n^{-3}\omega_0$, and the nuclear electric field is $F_n=n^{-4}F_0$. The scaled quantity used below is the ratio of the physical quantity and the atomic quantity.

II. METHOD OF CALCULATION

We describe the SSE under HCP by the following Hamiltonian:

$$\hat{H}=\frac{\hat{p}^2}{2}+\begin{cases}-1/z\pm zE_m\sin(\pi t/\tau) & \text{if } z>0\\ \infty & \text{if } z\leqslant 0,\end{cases} \tag{2}$$

where τ is the pulse duration. The $+$ sign indicates the electric field is polarized along the positive z axis and the $-$ sign for the reverse direction.

The system is prepared in an eigenstate with quantum number n before the turning on of the pulse. The wave function $\psi(z,t)$ in the time-dependent Schrödinger equation

$$i\frac{\partial\psi(z,t)}{\partial t}=\hat{H}\psi(z,t) \tag{3}$$

is propagated by the split-operator algorithm[10]

$$\psi(t+\Delta)=e^{-i\hat{p}^2\Delta/4}e^{-i\hat{V}\Delta}e^{-i\hat{p}^2\Delta/4}\psi(t)+O(\Delta^3), \tag{4}$$

where V is the potential in Eq. (2), and the effect of the operator $e^{-i\hat{p}^2\Delta/4}$ is evaluated by fast Fourier transform into the coordinate space.[10] The spatial range is taken from 0 to $25.6a_0$ using 512 evenly spaced grid points for the SSE initially prepared in the ground state, and 0 to $30\,720a_0$ using 2048 grid points for $n=100$. An absorbing function is placed near the outer boundary to prevent unphysical reflection.[11] For calibration, we propagate the system without external field to one-half Kepler cycle and calculate the sum over

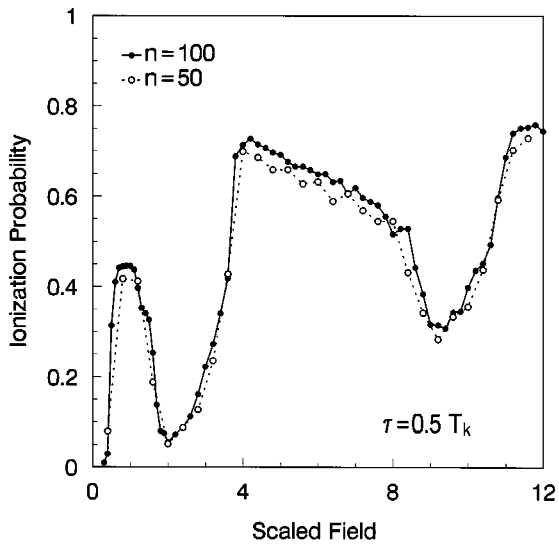

FIG. 1. Ionization probability against scaled field amplitude with field in the $+z$ direction. τ is the pulse duration and T_k is the Kepler period for state with quantum number n.

each grid for the squared deviation of calculated and exact wave functions. The deviation is less than 1% at the extremal case of $n=100$, about 50 times better for $n=1$. We are satisfied with the current accuracy though a finer grid will improve it. To obtain ionization probability, we project the wave function at the moment of the turnoff of the pulse to the WKB continuous wave function. For a positive energy ϵ, the normalized continuous wave function is

$$\phi_\epsilon(z)=\sqrt{\frac{2}{\pi p}}\sin\left[S_\epsilon(z)-\frac{\pi}{4}\right], \tag{5}$$

where the classical action function

$$S_\epsilon(z)=\int_0^z p(\xi)d\xi=pz+\frac{2}{\sqrt{2\epsilon}}\sinh^{-1}(\sqrt{\epsilon z}). \tag{6}$$

Equation (6) has the correct asymptotic behavior of Coulomb wave function. We calibrate the WKB solution with the unperturbed $\epsilon=0$ continuous wave of s wave in the three-dimensional Coulomb problem which has an available analytic solution.[12] For the ground state grid used, the sum over each grid for the squared deviation of WKB and analytic wave function is 0.22%, and is 0.17×10^{-3}% for the grid of $n=100$. So the WKB solution gives appropriate continuous wave function in this problem.

III. RESULTS AND DISCUSSIONS

In Fig. 1 we show the ionization probability of the highly excited surface-state electron against the scaled field ($F_s=n^4E_m$). The scaled field is directed along the $+z$ axis and lasts for one-half Kepler cycle. First, we observe that the ionization probabilities for $n=100$ and $n=50$ are nearly identical. This is consistent with the classical scaling behavior for high atomic Rydberg states.[13] Second, in the perturbative region (for scaled field $F_s<1$), the ionization probability increases with field amplitude. This is the region studied experimentally on atomic Rydberg states[1] and our

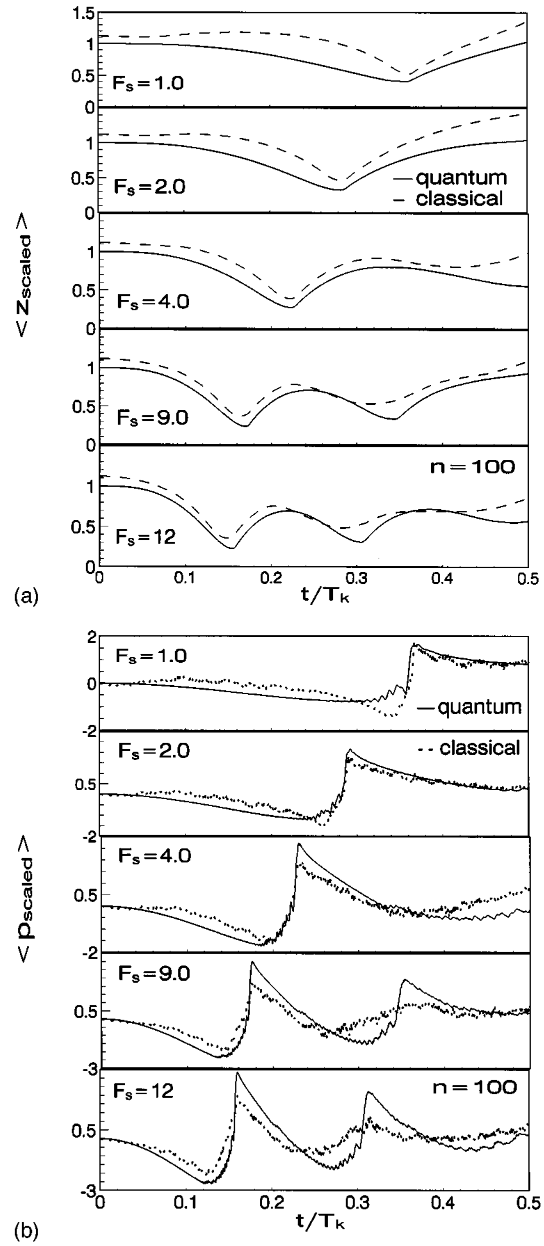

FIG. 2. (a) Average scaled coordinate against time with one-half Kepler period duration. (b) Average scaled momentum against time with one-half Kepler period duration.

results are consistent with experiment. Third, for fields in the nonperturbative region, the ionization probability shows anomalous stabilization windows as the fields are increased. The regime has not been investigated either in quantum calculations, or in experiment. A semiclassical calculation gave identical results.[14]

To understand the behavior shown in Fig. 1 for the HCP dynamics, we first look at the time evolution of the expectation values of the scaled position (z/n^2) and momentum (pn) at several specific scaled fields which show local extrema in Fig. 1. The results from the classical calculation are also shown. For the scaled field 1.0, in Fig. 2(a) the electron is first accelerated by both the external field and the Coulomb attraction due to the nucleus and it is ''bounced'' back at $0.36T_k$ by the wall at $z=0$. At the same time its momen-

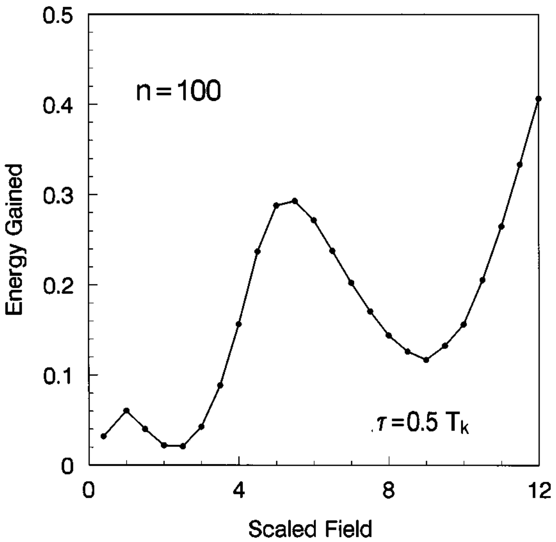

FIG. 3. Energy gained by the electron from the HCP pulse vs scaled field amplitude for field in the $+z$ direction with one-half Kepler period duration.

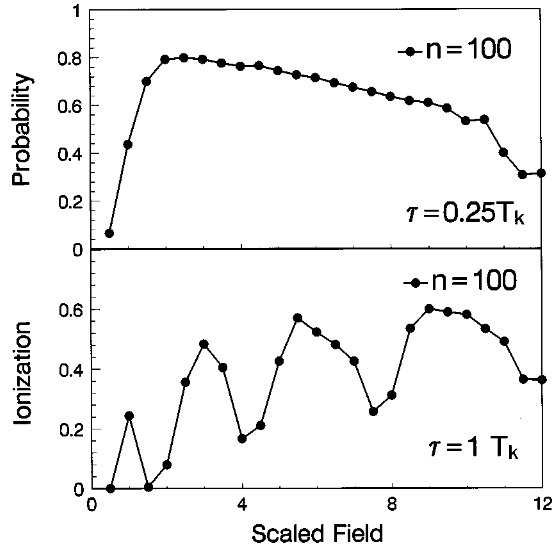

FIG. 5. Ionization probability against scaled field amplitude with field in the $+z$ direction for one-quarter and one Kepler period durations.

tum, as seen in Fig. 2(b), reverses the direction. As the electron moves out with certain momentum, the field is turned off at $0.5T_k$. The electron will then propagate without external force. We can see that the time scale is very important. For pulse with longer or shorter duration, the motion will be much different. When the field is increased, the bounce occurs at an earlier time as shown in the case of $F_s=2$ and 4. In the case of scaled field 9.0, the electron first bounces back at around $0.16T_k$. Near $0.25T_k$ (the electric field is at its maximum at the moment) it hits the barrier, due to the HCP electric field, and bounces back toward the nucleus. It gets another bounce by the nucleus at around $0.34T_k$. There is a similar behavior for the case of scaled field 12. Also shown in Fig. 2(a) and Fig. 2(b) are classical calculations. The classical results are obtained from a microcanonical ensemble of 500 initial conditions.[13] The quantum and classical results are quite close, which is expected for the highly excited surface-state electron that is considered.

Since the field is always directed in the $+z$ direction, the electron gains energy when moving toward $-z$ and loses energy when moving in the opposite direction. The total energy gained by the electron during the pulse is shown to determine the ionization probability. We mention that the classical energy gain was discussed in Ref. 1. The quantum mechanical energy gain is defined as

$$\text{Energy gained} = -\int_0^{\tau} E_m \sin(\pi t/\tau)\langle p(t)\rangle dt, \tag{7}$$

where $\langle p(t)\rangle$ is the quantum mechanical momentum expectation value at t. In Fig. 3 we plot the energy gained by the electron for each case described in Fig. 1. The energy gained

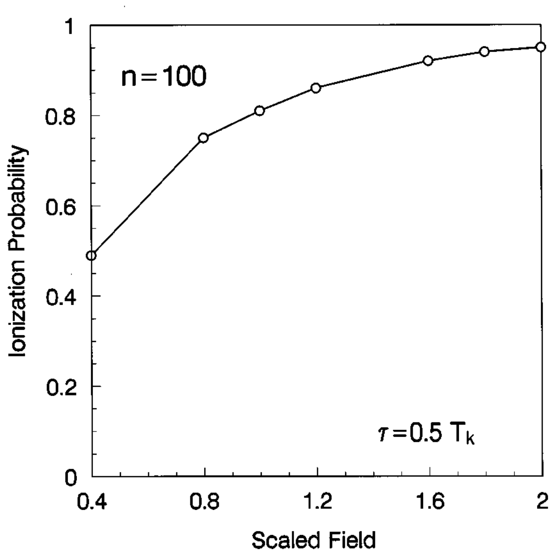

FIG. 4. Ionization probability against scaled field amplitude with field in the $-z$ direction with one-half Kepler period duration.

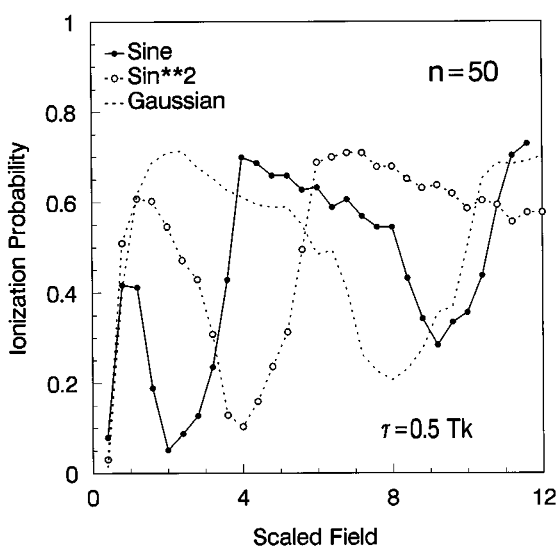

FIG. 6. Ionization probability of $n=50$ state with three different types of pulse shapes.

curve mimics the ionization probability and has the same characteristic local extrema at the same scaled fields as in Fig. 1. This justifies the interpretation that this quantity is the most critical factor in determining the ionization probability for the HCP dynamics.

For field directed along the $-z$ direction, the field always drives the electron away from the nucleus during the pulse. The stronger the field amplitude, the higher the ionization probability. Figure 4 depicts the results. The case is easy to understand and we did only one calculation.

For pulses with different duration, the oscillation of the ionization probability as seen in Fig. 1 also occurs. For a shorter pulse at $0.25T_k$, we expect less frequent oscillation. For a longer pulse, there will be more oscillations as the electron has the time to bounce back and forth between the wall at $z=0$ and the barrier due to the Stark field at positive z. The calculated results, as shown in Fig. 5, agree with this qualitative interpretation. We can expect that the longer the pulse duration, the more the number of windows will show up. In Fig. 6 we depict the effect of different pulse shapes on the ionization probability of the $n=50$ state. The pulse shapes used are $\sin(\pi t/\tau)$, $\sin^2(\pi t/\tau)$, and $\exp[-96(t/T_k-0.25)^2]$, where $\tau=0.5T_k$. The oscillation in ionization probability for each case is again determined by the energy gain.

IV. CONCLUSIONS

In summary, our simulation of the effect of a half-cycle pulse on a one-dimensional SSE based on the model Hamiltonian (2) has been shown to obtain ionization probability consistent with experimental measurement on high atomic Rydberg states in the low field regime. We have extended the calculation to the high scaled field regime and observed interesting oscillatory behavior of the ionization probability, if the polarization direction is directed away from the surface. The oscillation has been interpreted in terms of the energy gained by the electron as it bounces back and forth due to the wall at $z=0$ set in Eq. (2) and the barrier due to the Stark field from the pulse. Since the SSE Hamiltonian is a physical model, the stabilization windows would be interesting to measure.

ACKNOWLEDGMENTS

We are grateful for the cooperation of Professor Shih-I Chu's group in the initial stage. We also thank Professor Chii-Dong Lin for many instructive discussions. This work was supported by the National Science Council of Taiwan under Contract No. NSC-85-2112-M009-005, and US-TAIWAN cooperative research program.

[1] R.R. Jones, D. You, and P.H. Bucksbaum, Phys. Rev. Lett. **70**, 1236 (1993).
[2] R.R. Jones, N. E. Tielking, D. You, C. Raman, and P. H. Bucksbaum, Phys. Rev. A **51**, R2687 (1995).
[3] See, for example, M. Mallalieu and S.I. Chu, Chem. Phys. Lett. **258**, 37 (1996); K.J. LaGattuta and P.B. Lerner, Phys. Rev. A **49**, R1547 (1994); K.J. LaGattuta, *ibid.* **53**, 1762 (1996); A. Bugacov *et al.*, *ibid.* **51**, 1490 (1995); **51**, 4877 (1995).
[4] C.C. Grimes, T.R. Brown, M.L. Burns, and C.L. Zipfel, Phys. Rev. B **13**, 140 (1976); D.K. Lambert and P.L. Richards, *ibid.* **23**, 3282 (1981).
[5] R.V. Jensen, Phys. Rev. Lett. **49**, 1365 (1982); Phys. Rev. A **30**, 386 (1984); R.V. Jensen, J.G. Leopold, and D. Richards, J. Phys. B **21**, L527 (1988).
[6] J.E. Bayfield *et al.*, Phys. Rev. A **53**, R12 (1996); M.M. Sanders and R.V. Jensen, Am. J. Phys. **64**, 21 (1996); S.M. Susskind and R.V. Jensen, Phys. Rev. A **38**, 711 (1988).
[7] U.L. Pen and T.F. Jiang, Phys. Rev. A **46**, 4297 (1991); R. Dehnen and V. Engel, *ibid.* **52**, 2288 (1995).
[8] U.L. Pen and T.F. Jiang, J. Phys. B **28**, L69 (1995).
[9] T.F. Jiang and S.I. Chu, Chem. Phys. Lett. **240**, 278 (1995).
[10] M.R. Hermann and J.A. Fleck, Jr., Phys. Rev. A **38**, 6000 (1988); M.D. Feit, J.A. Fleck, Jr., and A. Steiger, J. Comput. Phys. **47**, 412 (1982).
[11] S.I. Chu and T.F. Jiang, Comput. Phys. Commun. **63**, 482 (1991).
[12] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics, Non-relativistic Theory*, 3rd ed. (Pergamon, Oxford, 1977), Sec. 36.
[13] J.G. Leopold and I.C. Percival, Phys. Rev. Lett. **41**, 944 (1978).
[14] S.I. Chu and M. Mallalieu (private communication).