Semiclassical model of the electron-impact ionization of hydrogen in the presence of a strong laser field

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Electron-impact ionization of hydrogen in the presence of a strong laser field is studied in the framework of the time-dependent Hartree-Fock theory. The probability distribution of the impact electron is further approximated by a plane circular disk, moving on a classical path along the polarization direction of the laser field. The remaining time-dependent Schrödinger equation for the hydrogen atom is solved numerically by finite-difference methods for different impact parameters, electron energies, and laser intensities. The integrated cross section for field-free impact ionization is found to agree remarkably well with previous results in the intermediate and high energy range (60–600 eV). Field ionization and collisional ionization can be simultaneously calculated with this model. [S1050-2947(99)03111-X]

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I. INTRODUCTION

Electron collisions play an important role in the context of optical field ionization of atoms by intense laser pulses. The importance of collisional interactions was recognized in such diverse fields as above threshold ionization [1], nonsequential double ionization [2], and inner-shell ionization [3,4]. In all these cases sequential field ionization alone cannot fully explain the ionization rates, energy spectra, and ion charge states observed.

In dense plasmas ionization dynamics is substantially dependent on many-particle effects, such as electron degeneracy, screening, and ion-ion correlations [5,6]. Coherence effects of multi-electron motion have also been proposed [7]. In the present work we will restrict attention to more rarefied media, where the model of binary electron-atom collisions becomes applicable. The theory of binary collisions must deal with two distinct features, the calculation of the ionization cross section and its averaging over the electron distribution. Both parts can be influenced by the laser field. The difference between cycle-averaged and thermal-averaged collisional-ionization rates has already been discussed in [8]. On the other hand, cross sections for laser-assisted collisions have been treated extensively in a series of papers (e.g., [9]), following the potential scattering formalism of Kroll and Watson [10], and a theory with dressed target states proposed by Byron and Joachain [11]. In most of these works, however, attention has been focused more on electron-atom scattering than target ionization. The existing work on laser-assisted electron-impact ionization gives a fairly complete account to electron-atom collisions, while it treats the laser-atom interaction in a perturbative manner only [12,13]. Therefore this approach appears to be most appropriate for the regime of field intensities below the field ionization threshold.

In the present work, we study electron-impact ionization of hydrogen in strong laser fields in the framework of the time-dependent Hartree-Fock theory (TDHF) [14,15]. This approach allows one to treat the time-dependent laser-atom interaction without approximations. Moreover, there exist accurate and efficient finite-difference methods for the solution of the one-particle time-dependent Schrödinger equation [16,17]. On the other hand, electron-atom collisions can only be treated in an approximate manner, mainly because correlation effects will be neglected. We therefore consider this approach as largely complementary to previous work on laser-assisted collisions.

In Sec. II, the present TDHF formulation of the collision problem is introduced and a simple regularized Coulomb-interaction for a circular homogeneously charged disk is proposed to account for collisions in the range of intermediate and high projectile energies. In the present framework, collisions are described in the space-time domain by an incident wave packet. To overcome some vagueness with respect to the shape and extent of the wave packet, we adopt a semiclassical viewpoint and consider the wave packet as a probability distribution of an ensemble of classical beam particles. Restricting attention to classical impact electrons, one can define the differential cross section without ambiguity as a function of the impact parameter and the particle energies. Furthermore, using an axially symmetric probability distribution for the beam electrons, one is able to exploit the cylindrical symmetry of the problem, which is not present in single particle collisions. In the approximation of uncorrelated particles, the classical ensemble average can be replaced by an average interaction potential, which is of the same form as the quantum-mechanical Hartree potential. Exchange correlations will be omitted in this approach.

In Sec. III, the numerical solution of the present collisional model is discussed and some results are presented. To validate the present procedure, electron-impact ionization of hydrogen in the absence of a laser field has first been studied, which represents a well-solved fundamental two-electron problem of atomic physics. It is noted, that an empirical formula for the experimental cross sections has been given in an early work by Lotz [18], but only in the last decade theoretical calculations [19–24] have satisfactorily reproduced the experimental results [25–27]. In particular, we mention the convergent close-coupling method of Bray and Stelbov-

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ics [22], which has achieved remarkably perfect agreement with measurements of Shah, Elliott, and Gilbody [25]. There have also been some attempts to solve the time-dependent Schrödinger equation numerically for two electrons by introducing restrictions to the electron-electron interaction in order to reduce the number of dimensions (Temkin-Poet models) [28–30]. Comparing the present semiclassical calculations with these results, excellent quantitative agreement for the total ionization cross section is obtained at intermediate and high energies. Discrepancies at low energies are expected due to the neglect of particle correlations.

Impact ionization in the presence of a laser field is discussed by comparing ionization probabilities at different laser intensities. It is found that the temporal evolution of field ionization can depend sensitively on collision events. Simple predictions prove only possible in the limit of low and high field intensities. At low intensities, the field ionization probability is enhanced by collisions, while it is dominated by field ionization alone at high intensities. It is noted that a qualitatively similar intensity dependence of the ionization probability can be observed in nonsequential double ionization of He [2].

The present collision model has obvious limitations. Correlation effects are neglected and a self-consistent quantum-mechanical calculation of the wave function of the impact electron was not attempted here. Nevertheless, the simplicity of the model makes it very attractive for computations, especially if more complex atoms are considered. The results of the model may serve as a useful guide for more elaborate treatments. In the present work atomic units will be used if not otherwise stated.

II. ELECTRON-IMPACT MODEL

In the present work, we consider the ionization of a hydrogen atom by electron impact in the presence of a laser field. The laser field will be described within the electric dipole approximation by a time-dependent electric field $\boldsymbol{F}(t)$ and the proton of the hydrogen atom is taken at rest at the origin of the coordinate frame. Denoting the coordinates and momenta of the two electrons by $\boldsymbol{q}_1$, $\boldsymbol{q}_2$ and $\boldsymbol{p}_1$, $\boldsymbol{p}_2$, respectively, the complete Hamiltonian of the three-body system is of the form,

$$H(\boldsymbol{p}_1,\boldsymbol{q}_1,\boldsymbol{p}_2,\boldsymbol{q}_2,t)=\sum_{i=1}^{2} H_e(\boldsymbol{p}_i,\boldsymbol{q}_i,t)+V_{ee}(\boldsymbol{q}_1,\boldsymbol{q}_2). \tag{2.1}$$

It is composed of a single electron Hamiltonian $H_e(\boldsymbol{p},\boldsymbol{q},t)$ for each electron and of the electron-electron interaction $V_{ee}(\boldsymbol{q}_1,\boldsymbol{q}_2)$. Using atomic units, H_e and V_{ee} are given by

$$H_e(\boldsymbol{p},\boldsymbol{q},t)=\frac{p^2}{2}-\frac{1}{q}+\boldsymbol{q}\cdot\boldsymbol{F}(t),$$
$$V_{ee}(\boldsymbol{q}_1,\boldsymbol{q}_2)=\frac{1}{|\boldsymbol{q}_1-\boldsymbol{q}_2|}. \tag{2.2}$$

The Hamiltonian (2.1) is the common starting point for both quantum-mechanical and classical treatments. Since the general two electron problem is a demanding task, a reduced description by single electron mean-field equations for uncorrelated particles is often desirable. The approximation of uncorrelated particles may be expected to be valid for fast collisions where the impact electron can be treated as an independent particle. We will briefly compare the mean field approach in quantum mechanics and classical mechanics and then introduce a semiclassical electron-impact model, which proves particularly well-suited for time-dependent calculations of collisions in the high and intermediate energy range.

A. Quantum-mechanical treatment

In quantum mechanics, the time-dependent Schrödinger equation for the two electron wave function $\psi(\boldsymbol{q}_1,\boldsymbol{q}_2,t)$ can be replaced within the framework of the time-dependent Hartree-Fock theory by a set of two equations for two single-electron orbitals $\phi_1(\boldsymbol{q}_1,t)$, $\phi_2(\boldsymbol{q}_2,t)$. Being mainly interested in a semiclassical treatment, we will neglect exchange correlations. The general TDHF equations [14,15] then reduce to,

$$i\frac{\partial\phi_1(\boldsymbol{q}_1,t)}{\partial t}=[H_e(\boldsymbol{p}_1,\boldsymbol{q}_1,t)+V_1^{eff}(\boldsymbol{q}_1,t)]\phi_1(\boldsymbol{q}_1,t), \tag{2.3a}$$

$$i\frac{\partial\phi_2(\boldsymbol{q}_2,t)}{\partial t}=[H_e(\boldsymbol{p}_2,\boldsymbol{q}_2,t)+V_2^{eff}(\boldsymbol{q}_2,t)]\phi_2(\boldsymbol{q}_2,t), \tag{2.3b}$$

where $\boldsymbol{p}=-i\boldsymbol{\nabla}$ is the momentum operator and the effective electron-electron interaction is given by self-consistent potentials of the Hartree form,

$$V_i^{eff}(\boldsymbol{q}_i,t)=\int d^3q_j V_{ee}(\boldsymbol{q}_i,\boldsymbol{q}_j)|\phi_j(\boldsymbol{q}_j,t)|^2, \quad i\neq j. \tag{2.4}$$

These equations can be solved with existing computational methods for the one-particle time-dependent Schrödinger equation. Initially, the wave function ϕ_1 may be taken to correspond to the hydrogen ground state and the wave function ϕ_2 to an incident wave packet. The first equation determines the evolution of the atomic electron in the presence of both an external laser field and an impact electron. Field ionization and collisional ionization are thereby treated on the same basis by time-dependent interaction potentials. The second equation describes laser-assisted scattering of the impact electron. The ionization and scattering processes are coupled by effective potentials. In the present treatment, we will restrict attention to an independent particle model, solving the first equation in the presence of a prescribed probability distribution for the impact electron only.

Although the TDHF equations may be solved for any sufficiently localized incoming wave packet, the modeling of a uniform flux of incoming electrons and the definition of the corresponding ionization cross section raises some conceptual difficulties. Apparently, the TDHF equations are not immediately applicable for an infinitely extended plane wave, since the self-consistent potential will diverge for this case. On the other hand, the shape and extent of localized wave packets will introduce some vagueness in the definition of the cross section. We therefore now adopt a classical view-

point, where collisions can be distinguished by their impact parameter and a unique choice for the probability distribution of the impact electron can be given.

B. Classical treatment

In classical statistical mechanics, a complete description of the system will be given by the two-particle distribution function $F(\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{p}_1,\boldsymbol{p}_2,t)$ in the six-dimensional phase-space of two electrons. The time evolution of the two-particle distribution function is governed by Liouville's equation

$$\frac{\partial F}{\partial t}+\sum_{i=1}^{2}\frac{\boldsymbol{\partial} H}{\boldsymbol{\partial} p_i}\cdot\frac{\boldsymbol{\partial} F}{\boldsymbol{\partial} q_i}-\frac{\boldsymbol{\partial} H}{\boldsymbol{\partial} q_i}\cdot\frac{\boldsymbol{\partial} F}{\boldsymbol{\partial} p_i}=0, \tag{2.5}$$

where i enumerates the particles. Ionization rates may be calculated directly from appropriate initial ensembles by particle simulations [31]. As in the quantum case, however, it is desirable to have simpler approximate descriptions in terms of a reduced one-particle distribution function

$$f_1(\boldsymbol{q}_1,\boldsymbol{p}_1,t)=\int d^3q_2d^3p_2F(\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{p}_1,\boldsymbol{p}_2,t) \tag{2.6}$$

for electron 1 and a corresponding function f_2 for electron 2. For plasma with many particles, it is well-known that the reduced distribution functions obey a set of statistical equations known as the BBGKY hierarchy [32]. For uncorrelated particles, the hierarchy can be truncated and the one-particle distribution function satisfies the Vlasov equation. Formally, the same method can be applied to the present two-electron problem. Integration of Eq. (2.5) over the phase space of particle 2 yields

$$\frac{\partial f_1}{\partial t}+\frac{\boldsymbol{\partial} H_e}{\boldsymbol{\partial} p_1}\cdot\frac{\boldsymbol{\partial} f_1}{\boldsymbol{\partial} q_1}-\frac{\boldsymbol{\partial} H_e}{\boldsymbol{\partial} q_1}\cdot\frac{\boldsymbol{\partial} f_1}{\boldsymbol{\partial} p_1}-\int d^3q_2d^3p_2\frac{\boldsymbol{\partial} V_{ee}}{\boldsymbol{\partial} q_1}\cdot\frac{\boldsymbol{\partial} F}{\boldsymbol{\partial} p_1}=0. \tag{2.7}$$

If the particles are assumed uncorrelated,

$$F(\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{p}_1,\boldsymbol{p}_2,t)=f_1(\boldsymbol{q}_1,\boldsymbol{p}_1)f_2(\boldsymbol{q}_2,\boldsymbol{p}_2), \tag{2.8}$$

the one-particle distribution function will satisfy the Vlasov-type equation,

$$\frac{\partial f_1}{\partial t}+\frac{\boldsymbol{\partial} H_e}{\boldsymbol{\partial} p_1}\cdot\frac{\boldsymbol{\partial} f_1}{\boldsymbol{\partial} q_1}-\frac{\boldsymbol{\partial}[H_e+V_1^{eff}]}{\boldsymbol{\partial} q_1}\cdot\frac{\boldsymbol{\partial} f_1}{\boldsymbol{\partial} p_1}=0, \tag{2.9}$$

with the average potential

$$V_1^{eff}(\boldsymbol{q}_1,t)=\int d^3q_2d^3p_2V_{ee}(\boldsymbol{q}_1,\boldsymbol{q}_2)f_2(\boldsymbol{p}_2,\boldsymbol{q}_2,t), \tag{2.10}$$

and an analogous equation holds for f_2. Taking the atomic electron to be represented by particle 1 and the impact electron by particle 2, it can be seen that the atomic ensemble actually evolves in the average potential of the beam particles in complete analogy with the nonexchange TDHF equations.

In classical mechanics, a proper choice of the distribution f_2 for a uniform beam of impact electrons can be found without ambiguity. For this purpose we will restrict attention to an axially symmetric geometry with cylindrical coordinates $(\varrho,\ \varphi,\ z)$. It is assumed that both the incident beam and the polarization direction of the laser field are directed along the z axis. This particular geometry will apply to the important case where the electrons are driven by the laser field and any transverse thermal motion can be neglected. Assuming a uniform flux j of beam particles at $z=-\infty$, the ionization rate due to electrons passing a surface element $dS=\varrho d\varrho d\varphi$ of the beam cross section can be written as

$$dr=p(\varrho,\varphi)jdS \tag{2.11}$$

where jdS is the number of electrons crossing dS per unit time and $p(\varrho,\varphi)$ is the ionization probability due to a single electron with collision parameter ϱ and azimuthal angle φ. The differential cross section for impact ionization is defined by

$$d\sigma=\frac{1}{j}dr=p(\varrho,\varphi)dS. \tag{2.12}$$

It is completely determined by the single-electron ionization probability $p(\varrho,\varphi)$. If the electron distribution of the atom is spherically symmetric or randomly oriented with respect to the incident electron, $p(\varrho,\varphi)$ will actually be independent of the angle φ. It is noted, however, that this symmetry will only hold in the average, since the Coulomb interaction

$$V_{ee}(\boldsymbol{q}_1,\boldsymbol{q}_2)=\frac{1}{|\boldsymbol{q}_1-\boldsymbol{q}_2|}=\frac{1}{\sqrt{\varrho_1^2+\varrho_2^2-2\varrho_1\varrho_2\cos(\varphi_1-\varphi_2)+(z_1-z_2)^2}} \tag{2.13}$$

depends explicitly on the angle difference $\varphi_1-\varphi_2$ between the impact electron and the atomic electron. To perform the angle average, it is therefore convenient to consider instead of a single impact electron an ensemble with definite values R for the impact parameter, Z for the z coordinate, and P for the momentum but with random angles,

$$f_2(\boldsymbol{p},\boldsymbol{q})=\delta(p_z-P)\,\delta(p_x)\,\delta(p_y)\frac{\delta(z-Z)\,\delta(\varrho-R)}{2\pi R}. \tag{2.14}$$

Due to the cylindrical symmetry, it will be sufficient to calculate the average ionization probability $\overline{p}(R)$ with respect to the ensemble (2.14). The total ionization cross section can be obtained from (2.12) by an integration with respect to the impact parameter,

$$\sigma_I=2\pi\int_0^\infty dR\,R\overline{p}(R). \tag{2.15}$$

In the present work, we will not attempt to calculate ionization probabilities by classical particle simulations. We rather wish to point out the basic conceptual framework for these calculations: The ionization cross section can be defined in terms of the ionization probability for a single point charge with impact parameter ϱ and azimuthal angle φ. Due to the cylindrical symmetry the ionization probability can be

calculated more easily for a statistical ensemble of incident particles with an axially symmetric probability distribution. Neglecting correlations between the beam and target electrons, the calculation of the ensemble averaged ionizaton rate $\overline{p}$ can be performed with the ensemble averaged interaction potential (2.10). In this manner, the basic dynamical equations become angle-independent and a close correspondence between the classical and the quantum-mechanical treatment of collisions can be established.

C. Semiclassical model

In the following, we will consider a semiclassical model for fast collisions. The semiclassial approach will be based on the TDHF equation (2.3a) for the wave function ϕ_1 of the atomic electron. The effective potential produced by the impact electron, however, will be modeled by an axially symmetric classical ensemble in a plane $z=Z(t)$ that moves along the z axis according to the classical equation of motion. Within this model, collisions can be well distinguished by their impact parameter R and the total ionization cross section for a uniform flux of incident particles can be obtained according to Eq. (2.15). Furthermore a simple closed form for a useful model potential can be gained.

The classical ensemble f_2, given by Eq. (2.14) corresponds to a homogeneously charged circular ring with radius R, centered at $z=Z(t)$ at time t and moving along the z axis with momentum $p_z=P$. Using Eqs. (2.13) and (2.14), the average potential (2.10) that is produced by this ring at time t at the position $(\varrho,\ \varphi,\ z)$ of the atomic electron is given by

$$V^{eff}_{ring}(\varrho,z,R,Z(t)) = \frac{1}{2\pi}\int_0^{2\pi}\frac{d\varphi_2}{\sqrt{\varrho^2+R^2+[z-Z(t)]^2-2\varrho R\cos(\varphi-\varphi_2)}} = \frac{K(m)}{\pi\sqrt{a+b}}, \tag{2.16}$$

where

$$a=\varrho^2+R^2+[z-Z(t)]^2,\quad b=2\varrho_1 R,\quad m=\frac{2b}{a+b}, \tag{2.17}$$

and $K(m)$ denotes the complete elliptic integral of the first kind. Due to the angle average, the potential becomes independent of φ. It is closely localized around the plane $z=Z(t)$. The radial profiles within the plane $z=Z(t)$ are represented in Fig. 1(a) for different values of the parameter R. One can see that the potential has a local minimum at $\varrho=0$, increases up to a maximum at the ring radius R and falls off rapidly beyond.

Numerical computations with the exact average potential (2.16) prove difficult, because it is strongly peaked at the ring radius. This singularity can only poorly be resolved on two-dimensional numerical grids with usual grid spacings. We therefore have chosen a model potential that keeps the main features of the exact potential while providing a regularization of the maxima. The smoothing is obtained by replacing the charge ring by a homogeneously charged circular disk with a density distribution,

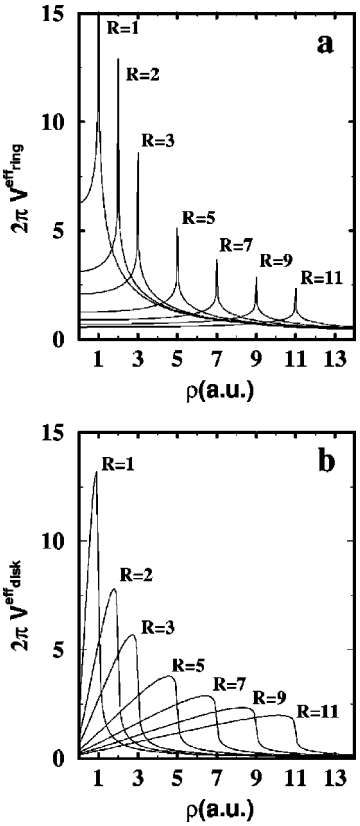

FIG. 1. Radial profiles of the average potentials $V^{\rm eff}$ produced by (a) a homogeneously charged circular ring of radius R, and (b) a homogeneously charged circular disk of radius R with modified Coulomb interaction. The potentials are represented in the plane of the charge distribution as a function of distance ϱ from the center. $V^{\rm eff}$, R, and ρ are expressed in atomic units.

$$\frac{1}{\pi R^2}\Theta(R-\varrho)\,\delta(z-Z), \tag{2.18}$$

where $\Theta(x)$ is the step function. Furthermore, in order to be able to perform the angular average in a closed form, the Coulomb interaction is replaced by a model interaction

$$V_{ee}=\frac{\delta(\varphi_1-\varphi_2)}{\sqrt{\varrho_1^2+\varrho_2^2-2\varrho_1\varrho_2\cos(\varphi_1-\varphi_2)+(z_1-z_2)^2}}, \tag{2.19}$$

acting only when both electrons have the same angular directions.

From this model a smooth average potential can be obtained in closed form,

$$V^{eff}_{disk}(\varrho,z,R,Z(t)) = \frac{1}{\pi R^2}\{\sqrt{[z-Z(t)]^2+(R-\rho)^2} - \sqrt{[z-Z(t)]^2+\rho^2}\} + \frac{\rho}{\pi R^2}\ln \times\left(\frac{R-\rho+\sqrt{[z-Z(t)]^2+(R-\rho)^2}}{-\rho+\sqrt{[z-Z(t)]^2+\rho^2}}\right). \tag{2.20}$$

Although this model potential appears less accurate from the physical viewpoint, it has the advantage that it provides one with a smooth and explicit representation for computations. Actually, the corresponding radial profiles, shown in Fig. 1(b) have the same qualitative behavior as those of the exact potential in Fig. 1(a), while avoiding the singular nature of the interaction.

III. NUMERICAL RESULTS

Based on the present semiclassical model, we have studied electron impact ionization of the hydrogen ground state for different impact parameters, particle energies, and laser intensities. For this purpose, the time-dependent Schrödinger equation (2.3a) with the average potential (2.20) has been solved numerically in cylindrical coordinates on a two-dimensional grid, by applying the Crank-Nicolson alternating-direction implicit method for time propagation. More details on the numerical procedure can be found elsewhere [16,17,33]. The calculations have been performed in atomic units with a time step of $\Delta t = 0.1$ a.u. and a spatial mesh size of $\Delta\varrho = \Delta z = 0.2$ a.u. The size of the numerical grid was chosen from $z = -80$ a.u. to $z = +80$ a.u. in the z direction and from $\varrho = 0.5\Delta\varrho$ to $\varrho = 80$ a.u. in the ϱ direction. In general, these values have been found sufficient for good convergence of the numerical solution. Initially, the atomic electron has been chosen to be in the ground state of the hydrogen atom and the incident electron has been initialized with kinetic energy $E = \frac{1}{2}P^2$ at the grid boundary $z = -80$ a.u.. The ionization probability has been defined as the probability to find the electron outside of a cylindrical volume V surrounding the atom,

$$p = 1 - \int_V dV |\phi_1|^2. \tag{3.1}$$

The size of this cylinder is chosen in such a way that it encloses a sphere of radius $r_a = 7$ a.u.

We first have calculated ionization cross sections for electron-impact ionization without a laser field. These cross sections can be compared with known experimental and theoretical results and thereby they provide a useful test on the limitations of the model. To determine the motion $Z(t)$ of the disk along the z axis, the equation of motion $\ddot{Z} = -\partial_Z V(Z)$ was solved for a one-dimensional screened Coulomb potential [34]

$$V(z) = -24.856 \frac{\exp(-\sqrt{z^2+16})}{\sqrt{(z^2+6.27^2)}}. \tag{3.2}$$

Since the deviations from the unperturbed ballistic motion are small, the details of this potential only play a minor role in our calculations. The evaluation of the ionization cross section as a function of energy requires a series of calculations of ionization probabilities for different impact parameters R and particle energies E. We have selected impact energies in the intermediate-high energy range, starting from the maximum of the cross section at about $E = 60$ eV up to $E = 600$ eV. Specifically, the values $E = 60$, 100, 150, 180, 200, 250, 300, 400, 500, and 600 eV have been chosen. For each energy, ionization probabilities have been calculated for the impact parameters $R = 0.2$, 0.5, 1, 2, 3, 5, 7, 9, and 11 a.u.. The total ionization cross section has been calculated according to Eq. (2.15) by integrating these probabilities with respect to R.

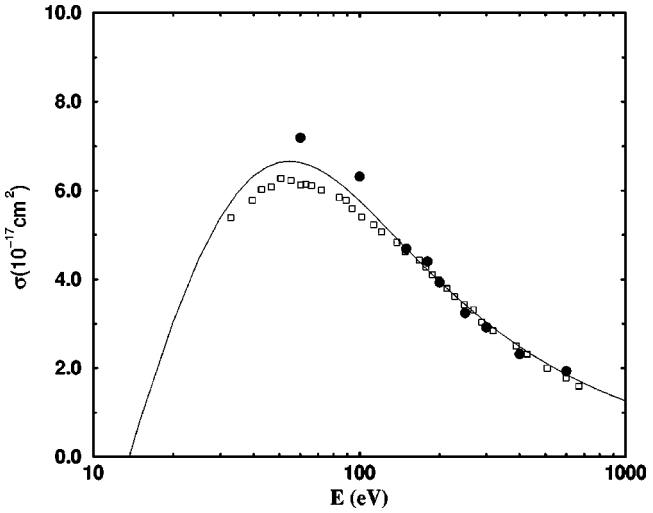

FIG. 2. Cross sections for electron-impact ionization of hydrogen as a function of the projectile energy. The results of the present semiclassical model (dots) are compared with the empirical formula of Lotz (solid line) and with experimental data from Shah *et al.* (squares).

In Fig. 2 cross sections calculated from this model are compared with the empirical formula of Lotz [18] and with the experimental results of Shah *et al.* [25]. For this comparison, the cross sections and the energies have been expressed in conventional units. We present results from 60 to 600 eV. One can see that the present model loses its validity below 60 eV. At lower energies, polarization and spin effects become important as well as the energy transfer to the incident electron. The ionization probabilities obtained beyond 600 eV become very small, and although they are inside the numerical precision, the cross sections can be less accurate. The most recent theoretical works correspond to the application of the convergent close coupling (CCC) method [22]. They give accurate ionization cross sections from threshold (13.6 eV) up to the high energy limit within the experimental error of Shah *et al.* We do not claim that our method is competitive with these almost exact *ab initio* results but, in view of the simplicity of the present collisional model, remarkably good agreement is obtained in the intermediate and high energy range.

Having validated the collisional model without a laser field, simultaneous field ionization by a time-dependent field, $F = F_0 \sin(\omega t)$, can be taken into account without further approximations. To demonstrate the effect of simultaneous field and collisional ionization, the most stringent case with maximum collisional cross section has been considered by choosing a fixed energy of $E = 60$ eV for the incident particle. In addition, a laser field with frequency $\omega = 0.2$ a.u. has been applied and the ionization probability has been calculated over a period of 5 optical cycles.

In Fig. 3, we compare ionization probabilities for field ionization with those obtained for field ionization with simultaneous collisions at three different impact parameters $R = 1$, $R = 2$, and $R = 7$ a.u. Ionization by electron impact

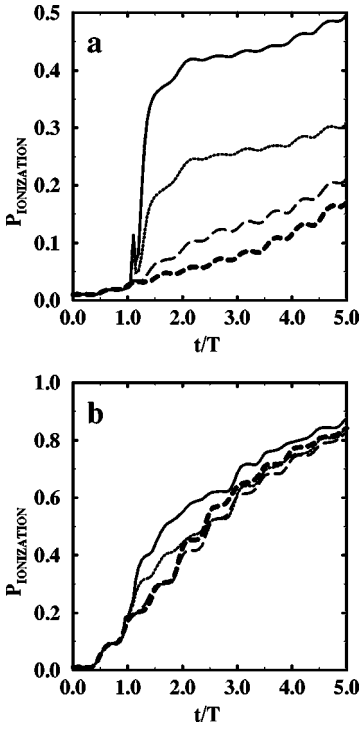

FIG. 3. Time evolution of ionization probabilities for field ionization with simultaneous collisions. The thick dashed lines correspond to field ionization in the absence of collisions for (a) a weak field with $\omega=0.2$, $F_0=0.05$, and (b) a strong field with $\omega=0.2$, $F_0=0.1$. The other lines, used when electron collisions are included, represent cases with impact parameter $R=1$ (solid line), $R=2$ (dotted line), and $R=7$ (dashed line). Electron impact takes place at time $t/T\approx 1$, where $T=2\pi/\omega$.

takes place in a short fraction of a laser cycle at $t/T\sim 1$, where T denotes the laser period, and its main feature is that it contributes with a sudden step to the time-dependent probability. The results in (a) correspond to a weak field with amplitude $F_0=0.05$ a.u. In this case, field ionization alone does not saturate and the effects of field and collisional ionization appear to be mainly additive. On the contrary, in (b) a stronger field with amplitude $F_0=0.1$ a.u. has been chosen. In this case field ionization reaches saturation during the calculation and all ionization curves approach the same limit. The total ionization probability can be well estimated by field ionization alone. However, looking at the details of the curves, one can see that collisions can significantly perturb the evolution of field ionization, giving rise to both higher and lower final ionization probabilities.

IV. CONCLUSION

The present study of electron-impact ionization has been based on a close correspondence between the quantum-mechanical and the classical mean-field treatments of collisions. This correspondence arises naturally when the classical particles are described by a probability distribution. Specifically, the quantum-mechanical TDHF equations correspond to classical Vlasov-type equations with the same form of the mean electron-electron interaction. We have considered a semiclassical approach, where the atomic electron is described quantum mechanically and the impact electron classically. Using an axially symmetric probability distribution for the incident particle, one is able to exploit the cylindrical symmetry of the collision problem, which is not expressed by the underlying three-body Coulomb Hamiltonian. Furthermore dealing with classical particles one can rigorously apply the impact parameter concept of the cross section. Approximating the probability distribution of the incident electron by a classically moving circular disk, a closed form for the collisional interaction could be obtained that can quantitatively reproduce electron impact ionization cross sections for hydrogen from intermediate up to high energies. The model has been applied to field ionization with simultaneous collisions and typical cases for the evolution of the ionization probabilities have been discussed. While the present work has concentrated on ionization probabilities for hydrogen, further studies of energy spectra and angular distributions might be adequate, since we expect that energies gained by the ionized electrons will be quite different when collisions are also included. An extension of these calculations to heavier atoms might also be of interest, although the inclusion of inner shell dynamics appears to be out of the scope of our present numerical procedure.

In summary, we have presented a model for fast laser-induced electron-atom collisions which allows one to calculate time-dependent collisions in the single-electron approximation.

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[1] G. G. Paulus, W. Nicklich, Huale Xu, P. Lambropoulos, and H. Walther, Phys. Rev. Lett. **72**, 2851 (1994).
[2] B. Walker, B. Sheehy, L. F. DiMauro, P. Agostini, K. J. Schafer, and K. C. Kulander, Phys. Rev. Lett. **73**, 1227 (1994).
[3] A. McPherson, B. D. Thompson, A. B. Borisov, K. Boyer, and C. K. Rhodes, Nature (London) **370**, 631 (1994).
[4] E. M. Snyder, S. A. Buzza, and A. W. Castleman, Jr., Phys. Rev. Lett. **77**, 3347 (1996).
[5] Y. T. Lee and R. M. More, Phys. Fluids **27**, 1273 (1984).
[6] H. Haberland and W. D. Kraeft, Phys. Rev. E **51**, 3459 (1995).
[7] B. D. Thompson, A. McPherson, K. Boyer, and C. K. Rhodes, J. Phys. B **27**, 4391 (1994).
[8] T. Ditmire, T. Donelly, A. M. Rubenchik, R. W. Falcone, and M. D. Perry, Phys. Rev. A **53**, 3379 (1996).
[9] P. Franken and C. J. Joachain, Phys. Rev. A **41**, 3770 (1990).
[10] N. M. Kroll and K. M. Watson, Phys. Rev. A **8**, 804 (1973).
[11] F. W. Byron, Jr. and C. J. Joachain, J. Phys. B **17**, L295 (1984).

[12] P. Martin, V. Véniard, A. Maquet, P. Francken, and C. J. Joachain, Phys. Rev. A **39**, 6178 (1989).
[13] D. B. Milošević and F. Ehlotzky, Phys. Rev. A **56**, 3879 (1997).
[14] K. C. Kulander, Phys. Rev. A **36**, 2726 (1987).
[15] C. Bottcher, G. J. Bottrell, and M. R. Strayer, Comput. Phys. Commun. **63**, 63 (1991).
[16] K. C. Kulander, Phys. Rev. A **35**, 445 (1987).
[17] M. S. Pindzola, G. J. Bottrell, and C. Bottcher, J. Opt. Soc. Am. B **7**, 659 (1990).
[18] W. Lotz, Z. Phys. **206**, 205 (1967).
[19] D. A. Konovalov and I. E. McCarthy, J. Phys. B **25**, L451 (1992).
[20] W. Hu, D. Fang, Y. Wang, and F. Yang, Phys. Rev. A **49**, 989 (1994).
[21] J. H. Macek, S. Yu Ovchinnikov, and S. V. Pasovets, Phys. Rev. Lett. **74**, 4631 (1995).
[22] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **70**, 746 (1993).
[23] K. Bartschat and I. Bray, J. Phys. B **29**, L577 (1996).
[24] T. T. Scholz, H. R. J. Walters, and P. G. Burke, J. Phys. B **24**, 2097 (1991).
[25] M. B. Shah, D. S. Elliot, and H. B. Gilbody, J. Phys. B **20**, 3501 (1987).
[26] T. W. Shyn, Phys. Rev. A **45**, 2951 (1992).
[27] G. O. Jones, M. Charlton, J. Slevin, G. Laricchia, A. Kover, M. R. Poulsen, and S. N. Chormaic, J. Phys. B **26**, L483 (1993).
[28] C. Bottcher, J. Phys. B **14**, L349 (1981).
[29] W. Ihra, M. Draeger, G. Handke, and H. Friedrich, Phys. Rev. A **52**, 3752 (1995).
[30] M. S. Pindzola and D. R. Schultz, Phys. Rev. A **53**, 1525 (1996).
[31] H. Schmitz, K. Boucke, and H.-J. Kull, Phys. Rev. A **57**, 467 (1998).
[32] N. N. Bogoliubov, *Studies in Statistical Mechanics*; edited by J. de Boer and G. E. Uhlenbeck (North-Holland, Amsterdam, 1962), Vol. I, p. 1.
[33] H.-J. Kull, L. Dimou, and J. L. Sanz, Laser Phys. **9**, 48 (1999).
[34] R. Grobe and J. H. Eberly, Phys. Rev. A **47**, 719 (1993).