Semiclassical Dirac Theory of Tunnel Ionization

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We present analytic tunnel ionization rates for hydrogenlike ions in ultrahigh intensity laser fields, as obtained from a *semiclassical* solution of the three-dimensional Dirac equation. This presents the first quantitative determination of tunneling in atomic ions in the relativistic regime. Our theory opens the possibility to study *strong laser field processes* with highly charged ions, where relativistic ionization plays a dominant role.

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The large progress in laser technology during the past decade has allowed the realization of laser pulses with peak intensities of 10^{21} W/cm^2 [1]. The next generation of laser sources will supply sub-10 fs pulses with peak intensities up to 10^{23} W/cm^2 [2]. At such intensities, ions up to charge states $Z = 50$–60 can be ionized. At near infrared laser intensities above 10^{18} W/cm^2, the motion of the electrons in a laser field becomes relativistic. Therefore, in the extreme parameter range accessible now by experiment, nonrelativistic tunnel ionization theories [3] are expected to break down. Currently, there exists no quantitative theory for relativistic tunnel ionization of atomic ions.

Field ionization is the primary process in matter exposed to high-intensity laser radiation, responsible for the generation of plasmas with energetic electrons and ions. The resulting particle dynamics is relevant for a wide range of research fields, such as atomic physics [4], astrophysics [5], plasma physics [6], and nuclear physics [7]. For example, the relativistic drift energy acquired by electrons during optical field ionization was utilized recently for the generation of sub-MeV to MeV electron bunches [8]. However, some of the observed photoelectron spectra exhibit features that are inconsistent with nonrelativistic ionization theory [9]. Understanding of this and other phenomena in the relativistic parameter regime makes a quantitative knowledge of optical field ionization indispensable.

The large potential for interesting applications has driven the quest for a theoretical understanding of relativistic optical field ionization. A 3D numerical solution of the Dirac equation in strong laser fields is prohibitively difficult [10], making analytical approaches necessary. Recently, an analytic solution of the Klein-Gordon equation for π^- atoms in static electric and magnetic fields was given [11]. In contrast to that, atomic ions were calculated by solving the Dirac equation [12,13] with exponential accuracy only, so far.

In this Letter, a quantitatively correct, semiclassical solution of the Dirac equation for relativistic field ionization of hydrogenlike ions is given. The analytic ionization rates go over into the ADK (Ammosov-Delone-Krainov) theory [3] in the nonrelativistic limit. The main difference between relativistic and nonrelativistic theory arises from the difference in binding energies, which starts to play a role for charge states $Z > 20$. The difference increases with increasing Z and becomes up to an order of magnitude for $Z = 60$. Ions with such charge states are generated at intensities between 10^{23} and 10^{24} W/cm^2.

The Dirac equation is solved in the relativistic system of units $c = m = \hbar = 1$, where c is the light velocity, m is the electron mass, and $\hbar$ is Planck's constant. Electron positron pair creation, arising in quantum electrodynamics, is negligible for the highest charge states ($Z = 60$) and laser intensities (10^{23} W/cm^2) investigated here. This is because the binding energy of 0.1 MeV for $Z = 60$ is much smaller than the energy gap between electron and positron continuum (≈ 1 MeV). Further, pair creation in vacuum takes place only at intensities close to the 6 orders of magnitude higher Schwinger intensity defined below.

The ground-state bispinor wave function for the hydrogenlike atom with charge Z is given by [14]

$$\Psi_{\rm gs} = \hat{S} B r^{\varepsilon - 1} \exp(-\mu r), \tag{1}$$

with quantum numbers $j = 1/2$, $m = 1/2$, $\kappa = -1$. Here, $r = \sqrt{x^2 + y^2 + z^2}$ and $\hat{S} = (s_1, s_2, s_3, s_4)$ is a bispinor with components $s_1 = \sqrt{1 + \varepsilon}$, $s_2 = 0$, $s_3 = -\sqrt{1 - \varepsilon}(z/r)$, and $s_4 = \sqrt{1 - \varepsilon}(x + iy)/r$. Further, $\mu = e^2 Z$ denotes the inverse of the Bohr radius $a_0 = 1/\mu$ and $B = 2^{\varepsilon - 1} \mu^{\varepsilon + 1/2} \sqrt{1/[\pi \Gamma(2\varepsilon + 1)]}$. Finally, the energy of the ground state ($Z < 137$), $\varepsilon = \sqrt{1 - \mu^2}$, can take values lying in the interval $0 < \varepsilon < 1$.

Our analysis of tunnel ionization is performed in the quasistatic approximation [1] and relies on the WKB theory [14]. The ground state (1) remains valid close to the nucleus, where the influence of the laser field is negligible. Far away from the nucleus, where the effect of the Coulomb potential is weak, the wave function is determined by a quasiclassical solution. A complete wave function can be constructed by matching of these two

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solutions. Matching must be done in the region $a_0 \ll z_0 \ll a$, where both solutions are valid. Here, $a = 3(\lambda^2 - 1)/2eF\lambda$ is the outer turning point [14], $\lambda = (1/2)(\sqrt{\varepsilon^2 + 8} - \varepsilon)$, e is the electron charge, and F is the laser electric field. The laser electric/magnetic field is assumed to be polarized in the z/y direction and to propagate in the x direction. In the quasistatic approximation, the electric and magnetic fields are assumed to be constant during the tunnel process. Further, the extension of the ionic ground state is much smaller than the laser wavelength, $a_0 \ll \lambda$, so that the laser electric and magnetic fields may be assumed spatially constant. Under these assumptions, the vector and scalar potential in the Lorenz gauge are found to be $\mathbf{A} = Fz\hat{\mathbf{x}}$ and $\varphi = Fz$ [15].

The quasiclassical solution is given by

$$\Psi_{\mathrm{qc}} = \hat{S}\frac{C}{\sqrt{p_z}}\exp\left(i\int_{z_0}^{z} p_z dz + i\int_{x_0}^{x} p_x dx + i\frac{\pi}{4}\right), \quad (2)$$

where p_z and p_x are the relativistic, canonical momenta in the direction of laser polarization and wave vector, respectively. The lower limits z_0 and x_0 denote the matching point. Note that in the presence of relativistic laser fields, the classical electron trajectory is two dimensional. The motion remains constant in the direction of the magnetic field, in which no force acts on the electron. Hence, the y direction may be omitted in the classical parts of our derivation.

Calculation of the quasiclassical momenta is done in two steps. First, the classical, canonical momenta p_{zc}, p_{xc}, and p_{yc} are determined. Approximation of the momenta in Eq. (2) by the classical momenta is sufficient to obtain the ionization rate with exponential accuracy. However, in order to determine the preexponential factor, in a second step, the classical momenta must be replaced by the quasiclassical momenta accounting for the quantum mechanical uncertainty around the classical trajectory. The classical canonical momenta are determined from the complex two-dimensional trajectory of the electron sub-barrier motion. The trajectory is obtained by a solution of the classical, relativistic equations of motion subject to the following boundary conditions: birth time $t = 0$, $z(t = 0) = a$, $z(t_0) = x(t_0) = 0$ with t_0 a complex time at which the electron energy is equal to the binding energy ε. The electron trajectories are found in terms of the parametric equations [11,15]

$$x = \frac{i}{2F\lambda}\left[(\lambda^2 - 1)u - \frac{1}{3}u^3\right],$$
$$z = \frac{1}{2F\lambda}[3(\lambda^2 - 1) - u^2], \quad (3)$$
$$t = \frac{i}{2F\lambda}\left[(\lambda^2 + 1)u - \frac{1}{3}u^3\right],$$

where $0 \le u \le \sqrt{3(\lambda^2 - 1)}$ is the parametric variable. The appearance of complex space coordinates, momenta, and times is associated with the classically forbidden sub-barrier motion of electrons. After the electron leaves the barrier, all quantities become real.

From Eq. (3) the total classical energy of the electron is found to be $E(u) = (\lambda^2 - u^2 + 1)/(2\lambda)$. The relativistic, classical canonical momentum is calculated by $p_{zc} = (dz/dt)E = i\sqrt{1 + P_{xc}^2 - (\varepsilon + eFz)^2}$, where $P_{xc} = E(dx/dt) = p_{xc} + eFz$ is the classical kinetic momentum in the x direction and the canonical momentum $p_{xc} = p_{x0} = p_{xc}(t_0) = (1/4)(3\varepsilon - \sqrt{\varepsilon^2 + 8}) < 0$ is equal to the initial x momentum at time t_0. Finally, $p_{yc} = 0$. The integral over dx in the quasiclassical wave function (2) gives no contribution, as p_{xc} is a constant and $x(t = t_0) = x(t = 0) = 0$. The remaining quasiclassical wave function (2), dependent only on the z integral, must be matched to the ground-state wave function. Finally, the quasiclassical momenta $p_x = p_{xc} + \delta p_x$ and $p_y = p_{yc} + \delta p_y$ are introduced that allow for a small deviation from the classical trajectories.

The constant C is determined by connecting Eq. (2) to the ground-state wave function. For that purpose, we perform a Fourier transformation of Eq. (1) with respect to the transverse coordinates x, y which results in

$$\Psi_{\mathrm{gs}}(z_0, \mathbf{p}_\perp) = \hat{S}\frac{2\pi B}{\tilde{p}_z}\exp(-\tilde{p}_z z_0 + \varepsilon \ln r_0). \quad (4)$$

Here, $\tilde{p}_z = \sqrt{p_{x0}^2 + \mu^2}$ denotes the momentum in the area left to the matching point, where F is negligible. Matching of Eq. (2) and of (4) yields the constant $C = (2\pi B/\sqrt{\tilde{p}_z})\exp(\varepsilon \ln r_0 - \tilde{p}_z z_0)$, so that the quasiclassical wave function under the barrier is completely determined.

In order to calculate the ionization rate, the exponentially decaying sub-barrier wave function is connected to the oscillating wave function on the right side of the outer turning point a [14] representing the ionized part of the electron wave function. By using $x, y \approx 0$ at $z \approx a$, we obtain

$$|\Psi_{\mathrm{qc}}(z > a, \mathbf{p}_\perp)| = \hat{S}\frac{2\pi B}{\sqrt{\tilde{p}_z}}\frac{1}{\sqrt{|p_z|}} \times \exp\left(-\int_0^a |p_z| dz + \varepsilon \ln r_0\right), \quad (5)$$

where the bispinor $\hat{S} \approx (\sqrt{1 + \varepsilon}, 0, -\sqrt{1 - \varepsilon}, 0)$. Calculation of the integral in Eq. (5) gives $\int_0^a p_z dz = (\mu^2 + p_\perp^2)^{3/2}/[3eF(\varepsilon - p_x)]$.

The integral $\int p_z dz$ was calculated by neglecting the Coulomb potential. To correct for that, we start from the quasiclassical wave function in the time domain, $Q = \exp(i\int \Delta E dt)$ that is equivalent to the space domain representation $\exp(i\int \mathbf{p} d\mathbf{r})$ with $d\mathbf{r} = (dx, dy, dz)$ used so far. This is because $\mathbf{p}d\mathbf{r} = \mathbf{p}\mathbf{v}dt = \Delta E dt$, where ΔE represents the change in energy caused by the presence of the Coulomb potential. By calculating the integral over the auxiliary variable ($dt = du[dt/du]$), the Coulomb correction is found to be

$$|Q|^2 = \left(\frac{2\xi^2(3-\xi^2)^{3/2}}{\sqrt{3}eF\sqrt{1+\xi^2}}\right)^{2\varepsilon}\exp\left(6\mu\arcsin\frac{\xi}{\sqrt{3}} - 2\varepsilon\ln r_0\right), \tag{6}$$

where $\xi = \sqrt{1-(1/2)\varepsilon(\sqrt{\varepsilon^2+8}-\varepsilon)}$.

The current is connected to the Coulomb corrected wave function by $j_z = p_z|Q\Psi_{\mathrm{qc}}(z>a, p_x, p_y)|^2$. Note that the arbitrary value of r_0 cancels out in j_z, in accordance with the requirements of WKB analysis [14]. By expanding p_x, p_y in the exponent around p_{xc}, p_{yc}, we obtain

$$j_z = \frac{8\pi^2B^2}{\tilde{p}_z}\left(\frac{2\xi^2(3-\xi^2)^{3/2}}{\sqrt{3}eF\sqrt{1+\xi^2}}\right)^{2\varepsilon}\exp\left(6\mu\arcsin\frac{\xi}{\sqrt{3}} - \frac{2\sqrt{3}\xi^3}{eF(1+\xi^2)} - A\delta p_y^2 - D\delta p_x^2\right), \tag{7}$$

with the expansion coefficients $A = \sqrt{3}\xi/(eF)$ and $D = \xi(\xi^2+3)/(\sqrt{3}eF)$. The parameter $\tilde{p}_z$ expressed in terms of ξ becomes $\tilde{p}_z = \sqrt{3}\xi/\sqrt{1+\xi^2}$. Equation (7) gives the transversal momentum distribution of the wave function at its time of birth in the continuum. The longitudinal momentum is determined by the fact that $p_z(z=a)=0$. The current is connected to the ionization rate by $w = 1/(2\pi)^2\iint j_z(\delta p_x, \delta p_y)d\delta p_x d\delta p_y$. Performing the integration over the transversal momenta results in

$$w_r = \frac{(eF)^{1-2\varepsilon}}{2\sqrt{3}\xi\Gamma(2\varepsilon+1)}\sqrt{\frac{3-\xi^2}{3+\xi^2}}\left(\frac{4\xi^3(3-\xi^2)^2}{\sqrt{3}(1+\xi^2)}\right)^{2\varepsilon}\exp\left(6\mu\arcsin\frac{\xi}{\sqrt{3}} - \frac{2\sqrt{3}\xi^3}{eF(1+\xi^2)}\right). \tag{8}$$

The tunnel ionization rate (8) can be transformed into SI or Gaussian units by making the following substitutions: $w_r \to w_r(mc^2/\hbar)$, $eF \to F/F_s$, and $\mu = e^2Z \to e^2Z/(\hbar c)$, where $F_s = m^2c^3/e\hbar = 1.32\times10^{16}$ V/cm is the Schwinger field strength [16] corresponding to an intensity $I_s = 4.7\times10^{29}$ W/cm^2. For the current in Eq. (7), the substitution $j_z \to j_z mc^3/\hbar$ must be made.

Equations (7) and (8) are the main result of this Letter, giving for the first time a quantitative description of tunnel ionization of atomic ions and of the resulting electron spectra. Tunnel ionization theory is valid in the so-called quasistatic or low frequency regime $\gamma \ll 1$, where

$$\gamma = \frac{\hbar\omega}{mc^2}\frac{F_s}{F}\sqrt{1-\left(\frac{\varepsilon}{mc^2}\right)^2} \tag{9}$$

denotes the relativistic generalization of the Keldysh parameter in Gaussian and SI units. In the nonrelativistic limit, γ reduces to the original Keldysh parameter [17]. In Eq. (9) ω denotes the circular frequency of the laser field.

In the remainder of this Letter, relativistic tunnel ionization of atomic ions will be characterized on the basis of Eq. (8). In order to be able to present data over a wide range of laser intensities, the ionization rates in Fig. 1 are plotted as a function of F/F_{bs}, where

$$F_{\mathrm{bs}} = \frac{F_s}{4\mu}(1-\sqrt{1-\mu^2})^2 \tag{10}$$

is the relativistic generalization of the barrier suppression field strength [18]. This is the field strength at which the maximum of the effective Coulomb barrier is equal to the binding energy, i.e., $V(z) = -\mu/z_m - eFz_m = \varepsilon - 1$. The position z_m, at which the barrier is maximum, is determined by $(d/dz)V(z) = 0$.

In Fig. 1(a) the *semiclassical* Dirac ionization rate (8) is depicted for various values of Z. The experimentally relevant range for tunnel ionization is between $0.3 < F/F_{\mathrm{bs}} < 0.7$. The upper limit is set by the fact that for $w_r \sim 1$ ionization is saturated within a fs.

Figure 1(b) shows the ratio of relativistic ionization rate w_r, Eq. (8), to the nonrelativistic ADK ionization rate w_{nr} [3]. For $Z=1$ the nonrelativistic and the relativistic theory agree, which corroborates the validity of our analysis. Note that for $F/F_{\mathrm{bs}} \to 0$, $w_r/w_{nr} \propto (F/F_{\mathrm{bs}})^{\mu^2} \to 0$, which comes from the difference between relativistic and nonrelativistic binding energy. However, the range $F \to 0$ is experimentally irrelevant as the ionization rate disappears. For $Z \geq 10$ relativistic effects start to appear. Up to $Z=20$ the difference between relativistic and nonrelativistic ionization theory is negligible within experimental accuracy. At $Z=40$ and 60 a deviation of up to a factor 3 and 10 appears in the experimentally relevant parameter regime.

The agreement between nonrelativistic and relativistic theory becomes better with increasing field strength. This, at first sight, counterintuitive behavior can be understood by recalling that there are two sources for relativistic effects: electron motion in the electromagnetic field (i) and in the nuclear potential (ii). As the distance under the barrier is extremely short and the electron is born with zero velocity in the continuum, (i) is expected to be weak. However, it is well known that for $Z \geq 10$ relativistic effects must be taken into account to model the ground-state wave function correctly [14]. For larger field strengths the laser field increasingly dominates the electron dynamics, as compared to the nuclear potential, which explains the increasingly better agreement found in Fig. 1(b).

In conclusion, an analytic, quantitative theory of tunnel ionization of atomic ions in relativistic laser fields was

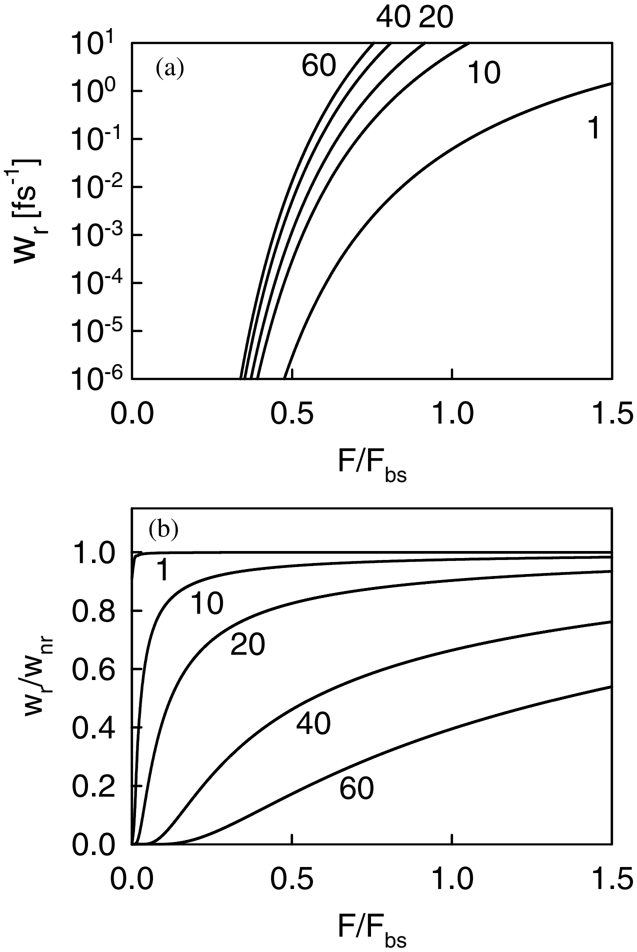

FIG. 1. (a) The relativistic ionization rate (8) for ionic charge states $Z = 1, 10, 20, 40, 60$. The field strength is normalized to the barrier suppression field strength, F_{bs}, given in Eq. (10). For $Z = 1, 10, 20, 40, 60$, the barrier suppression intensities are $I_{bs} = 1.4 \times 10^{14}$, 1.4×10^{20}, 9.0×10^{21}, 6.3×10^{23}, and 8.1×10^{24} W/cm^2, respectively. (b) The ratio of Dirac (w_r) to non-relativistic (w_{nr}) instantaneous ionization rates in an electromagnetic field.

derived. This gives quantitative, theoretical access to a new regime of plasma physics, where dynamical processes caused by ionization play a fundamental role. Here, we briefly discuss one example. It was demonstrated in recent experiments with laser intensities of a few times 10^{18} W/cm^2 that the (relativistic) drift energy acquired by electrons during ionization can be used for the generation of MeV electron pulses [8]. As the electron drift energy acquired at a Ti:S ($\lambda = 800$ nm) laser intensity of 10^{23} W/cm^2 is in the GeV range, this scheme holds the potential for the generation of single, ultrashort, highly directed, GeV electron pulses. A quantitative analysis of this process will be subject to further investigations, for which knowledge of Dirac tunnel ionization rates will be indispensable.

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