Coulomb-corrected strong-field approximation for the two-electron atom

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We present the model accounting for the Coulomb effects that occur in the direct double photoionization of the two-electron atom in an intense field of a circularly polarized plane wave. The model is the strong-field approximation (SFA) (the Reiss version of Keldysh-type models) applied to helium. We improve here our earlier study by inserting the electron-electron correlation in the initial state of the atom, and by inserting the Coulomb correction due to the influence of the nucleus on the final state of ionized electrons' pair. While the former improvement is of little significance, the latter extends the applicability range of the SFA (for typical laser wavelengths), and causes appreciable growth of the total ionization rate. [S1050-2947(97)00102-9]

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A single free electron oscillating in a plane-wave electromagnetic field is described by the Volkov or Gordon-Volkov [1,2] exact solution of the Schrödinger equation. This wave function was often applied in the models introduced by Keldysh, Faisal, and Reiss [3] to calculate the single-electron ionization of atoms by the strong laser field. There exists the analogous exact wave function [4] for two electrons interacting both mutually and with the laser field. This wave function has been employed in our calculations [5] of the direct double ionization of helium by the intense circularly polarized electromagnetic plane wave. In these calculations, as in the original Reiss approach [3], the influence of the remaining ion on the final state of ionized electrons has been neglected. Reiss and Krainov [6] have introduced an analytically simple dipole-approximation solution for the unbound electron in the simultaneous presence of the circularly polarized plane-wave laser field and a Coulomb potential. Their solution is simply the ordinary nonrelativistic Volkov state times temporal factor, which only makes a shift in energy. This Coulomb-corrected Volkov wave function well describes the electron, if the laser ''field is strong enough to require the unbound electron to move in a nearly circular orbit at a distance much larger than a Bohr radius from the center of the Coulomb force'' [6].

It is easy to derive a two-electron counterpart of the Coulomb-corrected Volkov state. The Schrödinger equation for two electrons in both the laser and nucleus Coulomb fields is

$$\left[i\frac{\partial}{\partial t} - \frac{1}{2}\left(-i\vec{\nabla}_1 + \frac{1}{c}\vec{A}(t)\right)^2 - \frac{1}{2}\left(-i\vec{\nabla}_2 + \frac{1}{c}\vec{A}(t)\right)^2 - V(\vec{r}_1,\vec{r}_2)\right]\Psi(\vec{r}_1,\vec{r}_2,t) = 0, \tag{1}$$

with

$$V(\vec{r}_1,\vec{r}_2) = -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r}. \tag{2}$$

(Atomic units are used throughout the paper.) $\vec{A}(t)$ is the vector potential for the circularly polarized plane-wave field in the dipole approximation, with the boundary condition $\lim_{t\to\pm\infty}\vec{A}(t)=\vec{0}$. Z is the charge of the nucleus, and the distance between the electrons is $r=|\vec{r}|=|\vec{r}_1-\vec{r}_2|$. We look for the approximate solution of Eq. (1) with a positive energy, i.e., when both electrons are not bounded by the atomic potential V. Our calculation is a straightforward generalization of that by Reiss and Krainov [6]. We introduce the Kramers-Henneberger [7,8] transformation for the two-electron wave function substituting

$$\Psi(\vec{r}_1,\vec{r}_2,t) = \exp\left(-i\int_{-\infty}^{t} d\tau A(\tau)^2 \Big/ c^2\right) \times \exp[\vec{\alpha}(t)\cdot\vec{\nabla}_1]\exp[\vec{\alpha}(t)\cdot\vec{\nabla}_2]\Phi(\vec{r}_1,\vec{r}_2,t), \tag{3}$$

with

$$\vec{\alpha}(t) = -\int_{-\infty}^{t} d\tau\vec{A}(\tau) \Big/ c. \tag{4}$$

Replacing the wave function Ψ in Eq. (1) by the right-hand side of (3), we get the equation satisfied by Φ. Performing algebraic operations included in the square brackets of Eq. (1) we get

$$\left[i\left(\frac{\partial}{\partial t}\right)_{\Phi} + \frac{1}{2}\nabla_1^2 + \frac{1}{2}\nabla_2^2 - V(\vec{r}_1,\vec{r}_2)\right] \times \exp\left(-i\int_{-\infty}^{t} d\tau A^2 \Big/ c^2\right)\exp(\vec{\alpha}\cdot\vec{\nabla}_1)\exp(\vec{\alpha}\cdot\vec{\nabla}_2)\Phi = 0, \tag{5}$$

where the differentiation over time acts only on Φ. Then we multiply Eq. (5) from the left-hand side by the product of two commutative operators: $\exp(-\vec{\alpha}\cdot\vec{\nabla}_1)\exp(-\vec{\alpha}\cdot\vec{\nabla}_2)$. Because both operators perform the well-known identity [6]

$$\exp(-\vec{\alpha}\cdot\vec{\nabla})V(\vec{r})\exp(\vec{\alpha}\cdot\vec{\nabla}) = V(\vec{r}-\vec{\alpha}), \tag{6}$$

we obtain

$$\left[i \frac{\partial}{\partial t} + \frac{1}{2} \nabla_1^2 + \frac{1}{2} \nabla_2^2 - V(\vec{r}_1 - \vec{\alpha}(t), \vec{r}_2 - \vec{\alpha}(t)) \right] \Phi(\vec{r}_1, \vec{r}_2, t) = 0. \quad (7)$$

For the circularly polarized plane wave the vector $\vec{\alpha}(t)$, from Eq. (4), only rotates, and its length is constant. We assume that the laser field (of frequency ω, electric-field amplitude F, and radiation intensity $I=2F^2$) is strong enough that

$$\alpha_0 \equiv |\vec{\alpha}(t)| = \frac{F}{\omega^2} \gg r_1, r_2. \quad (8)$$

Because we are going to incorporate the wave function Ψ in the S-matrix element with the helium atom ground state, r_1, r_2 should be limited to the values smaller than the radius r_z of the atom. It seems reasonable to define r_z as a radius of the sphere including both electrons with the probability of 90%, for example. If we employ the simple variational uncorrelated wave function with the effective nuclear charge of $Z_{\text{eff}}=Z-\frac{5}{6}$, e.g., [9], then we numerically obtain $r_z \cong 3.2/Z_{\text{eff}}$. (For the probability of 99% we have $r_z \cong 4.7/Z_{\text{eff}}$.) Thus, for helium we evaluate the lower radiation intensity limit (from the condition $\alpha_0 \geqslant 10 r_z$ with $Z=2$) to be about $7.2\times 10^2 \omega^4$. On the condition (8) Eq. (7) reduces to

$$\left[i \frac{\partial}{\partial t} + \frac{1}{2} \nabla_1^2 + \frac{1}{2} \nabla_2^2 - \left(-\frac{2Z}{\alpha_0} + \frac{1}{r} \right) \right] \Phi(\vec{r}_1, \vec{r}_2, t) = 0. \quad (9)$$

One solves the above equation by changing coordinates and the respective operators from $\vec{r}_1, \vec{r}_2, \vec{\nabla}_1, \vec{\nabla}_2$ to their center-of-mass and relative counterparts [4]:

$$\vec{R} = (\vec{r}_1 + \vec{r}_2)/2, \quad \vec{r} = \vec{r}_1 - \vec{r}_2, \quad (10)$$

$$\vec{\nabla}_R = \vec{\nabla}_1 + \vec{\nabla}_2, \quad \vec{\nabla}_r = (\vec{\nabla}_1 - \vec{\nabla}_2)/2.$$

The solution of Eq. (9), which is to describe two unbound electrons, may be parametrized either by their momenta $\vec{p}_1$, $\vec{p}_2$, or by their total and relative momenta $\vec{P}$, $\vec{p}$. Returning [through Eq. (3)] to the original wave function Ψ, we obtain the explicit approximate solution as the product of the repulsive Coulomb-wave function, satisfying the so-called ''ingoing'' boundary condition [9]:

$$\Phi_{\vec{p}}^{(-)}(\vec{r}) = \exp\left(-\frac{\pi}{4p} \right) \Gamma\left(1 - \frac{i}{2p} \right) \times \exp(i\vec{p}\cdot\vec{r}) F\left(\frac{i}{2p}, 1, -i(pr + \vec{p}\cdot\vec{r}) \right), \quad (11)$$

and the nonrelativistic Coulomb-corrected Volkov-type wave function

$$\Psi_{\vec{P}}^{CV}(\vec{R}, t) = \exp\left[i\vec{P}\cdot\vec{R} - i(P^2/4 + p^2)t + i\vec{\alpha}(t)\cdot\vec{P} - i \int_{-\infty}^{t} d\tau A^2(\tau) \Big/ c^2 + \frac{2iZ}{\alpha_0} t \right]. \quad (12)$$

In the above expressions $P=|\vec{P}|$, $p=|\vec{p}|$, Γ is Euler's gamma function, and F is the confluent hypergeometric function. Such a solution like $\Phi_{\vec{p}}^{(-)}$ has been chosen due to its application in the physical problem of ionization.

We have already employed the product of the similar wave functions as the final state of the outgoing electrons' pair in the direct double ionization of helium [5]. It is worth mentioning here the main idea of this paper. The following two-electron strong-field approximation (SFA) amplitude has been applied to describe the process

$$(S-1)_{fi} = -i \int dt (\Psi_{\vec{P}}^{V} \Phi_{\vec{p}}^{(-)}, H_I \Phi_i), \quad (13)$$

where $\Psi_{\vec{P}}^{V}$ is given by Eq. (12) without the last term in the exponent, $\Phi_{\vec{p}}^{(-)}$ is given by Eq. (11), $H_I(\vec{P}, t) = \vec{A}(t)\cdot\vec{P}/c + A(t)^2/c^2$ is the laser-atom interaction Hamiltonian in radiation gauge, and Φ_i is the laser-field-free initial atomic state (the helium atom ground state). Since the final state of the electrons' pair factorizes into two functions, one of the center-of-mass vector, and the other of the relative coordinate vector, it is convenient to calculate the sixfold spatial integral indicated by the parentheses of Eq. (13) in these variables. We have shown that a reasonable approximation of the initial state by the wave function, which depends only on the lengths of the above-mentioned vectors, enables us to reduce significantly the number of numerical spatial integrations to be done. The same mechanism works when we integrate the differential-ionization rate over all the possible final states of outgoing electrons.

In the present paper we employ our model to calculate the total direct double-ionization rate [Eq. (15)] of [5]), with two improvements. First, we apply a more accurate ground-state wave function including also the electron-electron radial correlation. This function has been constructed in a way similar to the one before [5], on the ground of the following wave function [10]:

$$\Phi_i(r_1, r_2, t) = N \exp(iE_B t)[\exp(-\alpha r_1 - \beta r_2) + \exp(-\alpha r_2 - \beta r_1)], \quad (14)$$

with $\alpha=2.179$, $\beta=1.189$, $E_B=2.904$, $N=0.7070$. The changes in the total ionization rate due to the better initial state increase with intensity from a few up to about 30%. Second, we apply the Coulomb-corrected Volkov final state (12) instead of the ordinary Volkov state. One can easily understand this change as a simple radiation frequency and intensity-dependent decrease of the binding energy

$$E_B(\omega, I) = E_B - 2\frac{Z}{\alpha_0(\omega, I)} = E_B - 2\sqrt{2}\frac{Z\omega^2}{\sqrt{I}}. \quad (15)$$

(For helium we have $E_B=2.904$ and $Z=2$.) In this expression intensity is bounded from below in such a way that for a given frequency the negative term is always much smaller than E_B. However, as we have observed previously [5], the SFA is quite sensitive to the value of the binding energy. Thus, even a small change in the binding energy may change the total ionization rate by a few orders of magnitude. (See Fig. 1.) It follows from Eq. (15) that in the limit of infinite

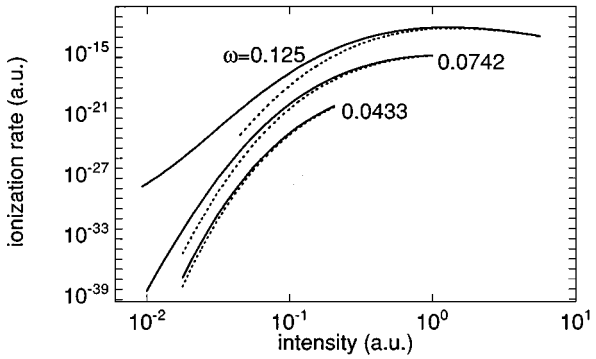

FIG. 1. The direct double-ionization rates for helium by the circularly polarized plane wave. Solid line, the Coulomb-corrected SFA; dotted line, the ordinary SFA. Frequencies are given in atomic units. $\omega=0.043$ a.u. corresponds to the wavelength of 1053 nm and $\omega=0.0742$ a.u. corresponds to the wavelength of 614 nm. For the intensity, 1 a.u. corresponds to 3.51×10^{16} W/cm^2.

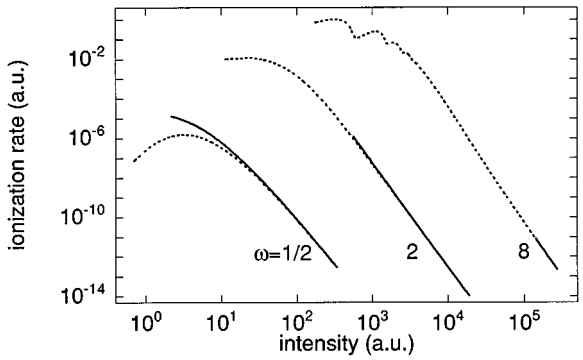

FIG. 2. As Fig. 1 for some higher frequencies. Each curve is shown for intensity starting from the ten times smaller one than the respective lower applicability limit.

intensity the second term vanishes, and we get the ordinary uncorrected SFA. Figures 1 and 2 show the direct double-ionization rate as a function of intensity for several frequencies. The ordinary SFA is supposed to be valid when $z_1\gg1$ [3]. The intensity parameter z_1 is equal to twice the ponderomotive potential U_p (of the ionized electron) divided by the electron binding energy (in the absence of the laser field). This condition applied here for the two-electron atom is $z_1\equiv4U_p/E_B\geqslant10$. Then the lower intensity limit is evaluated to be about $10\omega^2E_B$. The analogous limit for the Coulomb-corrected SFA has already been evaluated above. [See the text below Eq. (8).] While for higher frequencies including the Coulomb correction remarkably restricts the applicability range of the SFA (Fig. 2), for lower frequencies this range is extended (Fig. 1). The most important thing is the very high increase of the total ionization rate if the correction is taken into account.

However, our calculation indicates that the process described here is very weak for the intensities applied experimentally so far. There have been two experiments concerning the double ionization of helium by the strong circularly polarized laser field [11,12]. Fittinghoff *et al.* [11] have observed that the nonsequential rate, or the characteristic ''knee'' structure (on the plot of the He^{2+} ion counts) disappears when the polarization changes from linear to circular. Although a similar conclusion is made by Walker *et al.* [12], a slight ''knee'' shape may be recognized also in the case of circular polarization there (Fig. 3 of Ref. [12]). These authors suggest that the direct two-electron ionization seems to be the most logical explanation for helium.

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