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Approximation for a Coulomb-Volkov solution in strong fields

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A simple analytical approximation is found for the wave function of an electron simultaneously exposed to a strong, circularly polarized plane-wave field and an atomic Coulomb potential. The approximation is valid when $\alpha_0 \gg 1$, where α_0 is the classical radius of motion of a free electron in the plane-wave field. This constraint is sufficiently mild at low frequencies that it makes possible a major extension of the lower bound of laser intensities for which Volkov-solution-based approximations are useful.

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The Volkov or Gordon-Volkov [1,2] solution is an exact solution of the quantum-mechanical equations of motion for a free, charged particle in a plane-wave electromagnetic field. It has been applied in a variety of approximate procedures to calculate ionization of atoms [3–6], excitation in band-gap semiconductors [3,7], and laser-assisted scattering of electrons by atoms [8–10]. These applications could, in principle, be much strengthened and extended by the introduction of suitable corrections to the Volkov solution due to the presence of an atomic potential in addition to the plane-wave field. There have been previous efforts to incorporate such corrections [3,11–14]. They vary widely in nature, from *ad hoc* to detailed.

In this paper, we introduce an analytically simple dipole-approximation solution for an unbound electron in the simultaneous presence of a Coulomb potential and a circularly polarized plane-wave electromagnetic field. The solution is valid whenever the classical radius of motion α_0 of a free electron is large as compared to unity when only the circularly polarized field is present. (Atomic units are used here.) It is shown that this introduces corrections to the Volkov solution which allow very important extensions in the domain of validity for Volkov-based applications for all frequencies less than $\omega = 20^{-1/2}$ a.u. (when the application is to ground-state hydrogen). These frequencies include the entire current range of available strong lasers. The frequency constraint scales as $1/n^3$ for Rydberg states, where n is the principal quantum number. This is the same scaling that holds true for Rydberg frequencies in general.

The Schrödinger equation to be solved is

$$\left[i\partial_t - \frac{1}{2}\left(-i\nabla - \frac{A(t)}{c} \right)^2 - V(r) \right] \Psi(\mathbf{r},t) = 0. \tag{1}$$

Here, $\partial_t \equiv \partial/\partial t$, the fact that the vector potential of the plane-wave field is written as $\mathbf{A}(t)$ indicates that the dipole approximation is used, and atomic units are employed. The atomic binding potential is given by $V(r)$. The "space-translation" or Kramers-Henneberger [15–17] transformation is now introduced. This method has customarily been used [18] to describe an electron bound in an atom, subjected to a high-frequency field. We shall see that it is especially useful for the description of an unbound electron in a field of any frequency. To apply the Kramers-Henneberger transformation, we introduce a new function Φ, related to Ψ by

$$\Psi = \exp\left(-i \int_{-\infty}^{t} (A^2/2c^2)\, d\tau \right) \exp(\boldsymbol{\alpha}\cdot\nabla)\Phi, \tag{2}$$

where

$$\boldsymbol{\alpha}(t) = \int_{-\infty}^{t} \mathbf{A}(\tau)\, d\tau. \tag{3}$$

The boundary condition

$$\lim_{t \to \pm\infty} \mathbf{A}(t) = \mathbf{0}$$

is applied to the electromagnetic field. Using the Baker-Hausdorff theorem, we find the well-known result that

$$e^{-\boldsymbol{\alpha}\cdot\nabla} V(\mathbf{r}) e^{\boldsymbol{\alpha}\cdot\nabla} = V(\mathbf{r} - \boldsymbol{\alpha}). \tag{4}$$

Equations (1)–(4) give the equation satisfied by Φ as

$$[i\partial_t - \tfrac{1}{2}(-i\nabla)^2 - V(|\mathbf{r} - \boldsymbol{\alpha}(t)|)]\Phi = 0. \tag{5}$$

Equation (5) is exact within the constraints of the dipole approximation already specified, and applies to any potential $V(r)$. We consider here the special case of the Coulomb potential $V(r) = -Z/r$, where Z is the number of charges on the atom or ion, which gives

$$V(|\mathbf{r} - \boldsymbol{\alpha}(t)|) = -\frac{Z}{|\mathbf{r} - \boldsymbol{\alpha}(t)|}. \tag{6}$$

It must be remembered that the physical problem at hand is one in which the electron is in a positive-energy (i.e., unbound) state. We presume that the plane-wave field is strong enough that

$$\alpha_0 \gg 1/Z, \tag{7}$$

where α_0 is the radius of the circular classical motion of a free electron in a circularly polarized field. When the Coulomb-corrected Volkov state is incorporated into a matrix element with a bound state, as it will be, for example, in the calculation of photoionization, then the magnitude of $\mathbf{r}$ will be such that $|\mathbf{r}| \leq a_0/Z \equiv 1/Z$, where a_0 is the Bohr radius. This limit, in association with the condition (7), leads directly to the approximation

$$V(|\mathbf{r}-\boldsymbol{\alpha}(t)|) \approx -\frac{Z}{|\boldsymbol{\alpha}|} = -\frac{Z}{\alpha_0}. \tag{8}$$

Physically, this means that the 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. The approximation in Eq. (8) has two important consequences. One is that the modified form of Eq. (5) has the simple solution

$$\Phi \approx C \exp\left[i\left(\mathbf{p}\cdot\mathbf{r} - \frac{p^2}{2}t + \frac{Z}{\alpha_0}t \right) \right], \tag{9}$$

where C is a normalization constant and $\mathbf{p}$ is a constant vector. The second consequence is that this approximate solution for Φ is an eigenfunction of the operator in Eq. (2). The result for the Coulomb-corrected Volkov solution is then

$$\Psi \approx C \exp\left[i\left(\mathbf{p}\cdot\mathbf{r} - \frac{p^2}{2}t \right) \right] \exp\left[i\int_{-\infty}^{t} d\tau \left(\frac{\mathbf{p}\cdot\mathbf{A}}{c} - \frac{A^2}{2c^2} \right) \right] \times \exp\left(i\frac{Z}{\alpha_0}t \right). \tag{10}$$

The first two exponential factors in Eq. (10) constitute the usual nonrelativistic Volkov solution. The last exponential is the correction due to the presence of the Coulomb potential in this strong-field, unbound, circular-polarization case.

We note that the Coulomb-Volkov solution in Eq. (10) differs from an ordinary Volkov solution only by a simple shift in energy, so that the absolute square of the wave function and the expectation values of arbitrary functions of $\mathbf{r}$ and $\mathbf{p}$ are the same for Coulomb-Volkov solutions as for Volkov solutions. However, exactly the same thing can be said of a comparison of Volkov solutions with simple free-particle solutions. The important thing is that the energy difference between Coulomb-Volkov and Volkov solutions leads to significantly different dynamical predictions. For example, the transition amplitudes employed in the strong-field approximation (SFA) [5,19] would be revised from

$$(S-1)_{fi}^{v} = -i\int_{-\infty}^{\infty} dt(\Psi_f^v, H_I\Phi_i) \tag{11}$$

to

$$(S-1)_{fi}^{cv} = -i\int_{-\infty}^{\infty} dt(\Psi_f^{cv}, H_I\Phi_i), \tag{12}$$

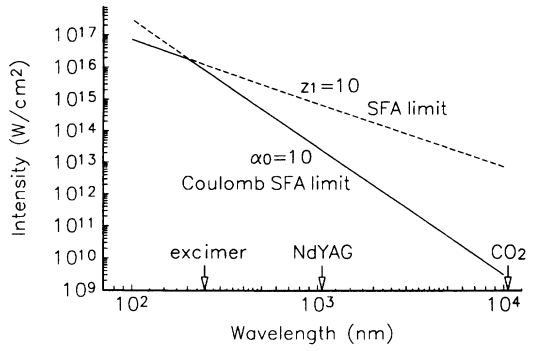

FIG. 1. The straight line labeled $z_1=10$ is the lower limit of applicability for the Volkov solution as applied in the SFA method. The line labeled $\alpha_0=10$ is the corresponding limit for the Coulomb correction to the Volkov solution as employed in the SFA. Since these lines cross, the solid line is the final applicability limit for the Coulomb-corrected SFA; that is, the region above and to the right of the solid line is accessible to description by the Coulomb SFA. The arrows on the wavelength axis mark the locations of several important available laser frequencies.

where here Φ_i is the laser-field-free initial atomic state. In the long-pulse approximation, where energy conservation is approximately true, the energy conservation conditions associated with Eqs. (11) and (12) are different. The correspondence between them can be stated either as $U_p \rightarrow U_p - Z/\alpha_0$, or as $E_B \rightarrow E_B - Z/\alpha_0$, where U_p is the ponderomotive potential experienced by the unbound electron in the laser field, and E_B is the binding energy experienced by the bound atomic electron.

To appraise the practical significance of the condition (7), Fig. 1 is presented for the case $Z=1$. This shows the limitations imposed by the restriction $\alpha_0 \geq 10$, expressed as a relationship between laser intensity in W/cm^2 and laser wavelength in nanometers. The same figure also shows the constraint $z_1 \geq 10$, which is the strong-field limitation inferred [19] for the application of Volkov-based methods like the SFA [5,19] for atomic photoionization. The quantity z_1 is the ratio of twice the ponderomotive potential of an electron in the laser field to the binding energy of the atom from which ionization takes place. The quantities α_0 and z_1 are given (in a.u.) for circular polarization in terms of laser electric field amplitude F and frequency ω by

$$\alpha_0 = \frac{F}{\omega^2}, \tag{13}$$

$$z_1 = \frac{(F/\omega)^2}{E_B}, \tag{14}$$

where E_B is the no-field atomic binding energy.

The condition $z_1 \gg 1$ implies that the behavior of the electron is dominated by the laser field, rather than the atomic field. Figure 1 shows that $\alpha_0 \geq 10$ is a milder condition than $z_1 \geq 10$ for frequencies below $\omega = 20^{-1/2}$ a.u. (or wavelengths longer than 204 nm), when the z_1 parameter refers to the binding energy of ground-state hydrogen. This crossover point follows from Eqs. (13) and (14) with $\alpha_0=10$, $z_1=10$. By the time wavelengths as long as 10 μm are

reached, the enlargement of the region of applicability made possible by the Coulomb correction amounts to between three and four orders of magnitude in laser intensity, corresponding to a change from a lower limit of 7×10^{12} W/cm^2 to a new lower limit of 3×10^{9} W/cm^2.

For a hydrogenic Rydberg state of principal quantum number n, the condition in Eq. (7) should be replaced by $\alpha_0 \gg n^2/Z$. The binding energy $E_B=Z^2/(2n^2)$ employed in the definition of z_1 gives $z_1=2(nF/Z\omega)^2$. Hence the crossover for the constraint on Volkov-state applicability given by $z_1 \geq 10$ to one given by $\alpha_0 \geq 10n^2/Z$ occurs for

$$\omega \leq \frac{Z^2}{20^{1/2}n^3}. \tag{15}$$

The $1/n^3$ frequency behavior in Eq. (15) is the same as that which obtains generally for Rydberg scaling of frequencies.

A specific example of the application of Eq. (10) is given in Fig. 2, which shows a comparison between the conventional SFA in the stabilization regime [20] and the Coulomb-corrected version of the same calculation at the experimentally important frequency of $\omega=0.043$ a.u. ($\lambda=1.06$ μm). Figure 2 is for $Z=1$, $n=1$. The considerable extension to lower intensities afforded by the restriction $\alpha_0 \geq 10$ in place of $z_1 \geq 10$ is in evidence, as well as the fact that the Coulomb interaction significantly enlarges the transition rate at the low end of the allowed range. Furthermore, the Coulomb-corrected result serves to substantiate the $z_1 \geq 10$ restriction previously inferred [19] for the uncorrected SFA.

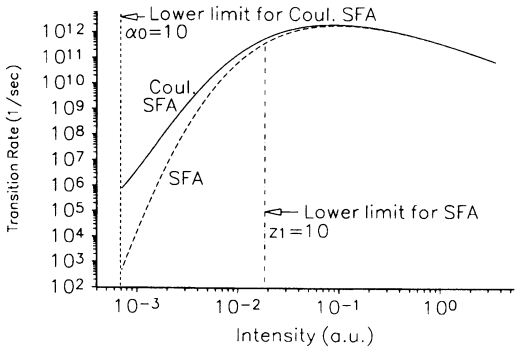

FIG. 2. An example of the application of the Coulomb-corrected Volkov solution in the SFA method to photoionization from the ground state of hydrogen by circularly polarized light of wavelength $\omega=0.043$ a.u. ($\lambda=1.06$ μm). The dash-dotted line ($z_1=10$) marks the lower intensity limit of applicability for the ordinary SFA, and the short-dashed line ($\alpha_0=10$) shows the considerable extension made possible through Coulomb corrections to the Volkov solution. In both cases, the stabilization phenomenon is clearly visible. Note that the rate curves for the SFA and Coulomb SFA become substantially coincident at $z_1=10$.

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