Comment on "Approximation for a Coulomb-Volkov solution in strong fields"

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We show that the derivation of the approximate solution for the motion of an unbound electron in the simultaneous presence of the Coulomb field and a circularly polarized plane wave given in Reiss and Krainov Phys. Rev. A **50**, 910(R) (1994) contains an error caused by confusing the space coordinates before and after the Kramers-Henneberger transformation.

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In [1], an attempt was made to derive a simple approximate solution for an unbound electron in the simultaneous presence of Coulomb and circularly polarized laser fields. In the present Comment, we shall show that the derivation of [1] contains an error that, quite surprisingly, not only seems to have escaped notice so far but has also been repeated in some publications in which "generalizations" of the derivation of [1] were proposed.

For convenience, we start by repeating in some detail the derivation given by the authors of [1]. They begin with the Schrödinger equation for an electron moving in the presence of the atomic (Coulomb) potential and the field of a circularly polarized monochromatic electromagnetic wave,

$$i\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=\left[\frac{1}{2}\left(\hat{\mathbf{p}}+\frac{1}{c}\mathbf{A}(t)\right)^2+V(r)\right]\Psi(\mathbf{r},t). \tag{1}$$

In the above equation, $\mathbf{r}$ and $\hat{\mathbf{p}}=-i\boldsymbol{\nabla}$ are the coordinates and (canonical) momentum operator, respectively, for the electron. Further, $V(r)$ is the atomic potential, $\mathbf{A}(t)$ [with $\mathbf{A}(t\rightarrow-\infty)\rightarrow 0$] is the vector potential of the wave field taken in the dipole approximation, and c is the speed of light. Atomic units are used.

The authors of [1] are especially interested in the motion of an unbound electron and, in order to find an approximate solution for this motion, introduce the Kramers-Henneberger transformation [2]. This transformation consists of expressing the wave function Ψ via a new function Φ according to

$$\Psi(\mathbf{r},t)=\exp\left(-i\int_{-\infty}^{t}A^2/2c^2dt'\right)\exp(\boldsymbol{\alpha}\cdot\boldsymbol{\nabla})\Phi(\mathbf{r},t), \tag{2}$$

where $\boldsymbol{\alpha}(t)=-\frac{1}{c}\int_{-\infty}^{t}\mathbf{A}(t')dt'$. By inserting Eq. (2) into Eq. (1) and multiplying from the left both sides of the resulting equation by the operator $\exp(-\boldsymbol{\alpha}\cdot\boldsymbol{\nabla})$, one obtains

$$i\frac{\partial}{\partial t}\Phi(\mathbf{r},t)=\left[\frac{1}{2}\hat{\mathbf{p}}^2+V(|\mathbf{r}-\boldsymbol{\alpha}|)\right]\Phi(\mathbf{r},t), \tag{3}$$

where in the case of the Coulomb atomic potential

$$V(|\mathbf{r}-\boldsymbol{\alpha}|)=-\frac{Z}{|\mathbf{r}-\boldsymbol{\alpha}|} \tag{4}$$

with Z being the charge of the atomic nucleus (atomic core). Up to now the consideration of [1] followed the standard lines repeated many times in the literature.

If the interaction V in Eq. (3) is neglected, the solution of Eq. (3) is a plane wave which, after inserting into Eq. (2), transforms into the well known nonrelativistic Volkov solution for a free electron in the field of a circularly polarized plane wave. The authors of [1] want to obtain a Coulomb correction to the Volkov solution. To this end, they first remark that for laser fields strong enough one has $\alpha_0=|\boldsymbol{\alpha}(t)|\gg 1/Z$, where α_0 represents the radius of a circular motion of a free (classical) electron in a circularly polarized wave [3] and $1/Z$ is the typical size of the atomic ground state. Further, the authors note that the solution they want to derive is to be incorporated into a transition matrix element with the ground state, and, therefore, electron-nucleus distances of importance for the transition amplitude will typically be of the order or less than $1/Z$. As a result, they argue that in Eq. (3) one can set

$$V(|\mathbf{r}-\boldsymbol{\alpha}|)\approx-\frac{Z}{|\boldsymbol{\alpha}|}=-\frac{Z}{\alpha_0}. \tag{5}$$

The approximation (5) is the key step in the consideration given in [1]. Once this step has been made, the derivation of the approximate solution becomes straightforward and yields this solution as

$$\Psi_{\mathrm{RK}}=\exp\left[i\left(\mathbf{k}\cdot\mathbf{r}-\frac{k^2}{2}\right)\right]\exp\left[i\int_{-\infty}^{t}\left(\frac{\mathbf{k}\cdot\mathbf{A}}{c}-\frac{A^2}{2c^2}\right)dt'\right]\times\exp\left(i\frac{Z}{\alpha_0}t\right), \tag{6}$$

where $\mathbf{k}$ is the electron momentum. Equation (6) is simply a product of the Volkov solution and the Coulomb correction factor $\exp\left(i\frac{Z}{\alpha_0}t\right)$. In [1], the wave function (6) is termed the Coulomb-Volkov solution. Equation (6) is the main result of [1].

Let us now point out that, while it is certainly true that the main contribution to the transition matrix element is given by the region of small electron-nucleus distances where the atomic ground state is located, this observation is by no means a justification for the approximation (5) to be valid.

First, note that it is the state $\Psi(\mathbf{r},t)$ given by Eq. (2) [but not the function $\Phi(\mathbf{r},t)$ from Eq. (3)] that directly enters the transition matrix element with the atomic ground state. Let us assume for the moment that we were able to find the exact solution of Eq. (3), $\Phi_{\mathrm{ex}}(\mathbf{r},t)$. Inserting this solution into Eq. (2) and taking into account that the action of the operator $\exp(\boldsymbol{\alpha}\cdot\boldsymbol{\nabla})$ is just to shift $\mathbf{r}$ in $\Phi_{\mathrm{ex}}(\mathbf{r},t)$ by $\boldsymbol{\alpha}$, we obtain

$$\Psi(\mathbf{r},t) = \exp\left(-i\int_{-\infty}^{t} A^2/2c^2 dt'\right)\exp(\boldsymbol{\alpha}\cdot\boldsymbol{\nabla})\Phi_{\mathrm{ex}}(\mathbf{r},t)$$
$$= \exp\left(-i\int_{-\infty}^{t} A^2/2c^2 dt'\right)\Phi_{\mathrm{ex}}(\mathbf{r}+\boldsymbol{\alpha},t). \quad (7)$$

From the second line of Eq. (7) it is obvious that in the region $r \lesssim 1/Z$, which is the only region where the state $\Psi(\mathbf{r},t)$ may have a substantial overlap with the initial (ground) atomic state and which is thus most important for the transition matrix element, the absolute value of the space argument of the function $\Phi_{\mathrm{ex}}(\mathbf{r}+\boldsymbol{\alpha},t)$ at $\alpha_0 \gg 1/Z$ is in fact close to α_0 and not to $1/Z$. But this means that in Eq. (3) the region of $\mathbf{r}$, which is most important for the transition matrix element, is given not by $|\mathbf{r}| \lesssim 1/Z \ll \alpha_0$ but by $\alpha_0 - 1/Z \lesssim |\mathbf{r}| \lesssim \alpha_0 + 1/Z$, where $|\mathbf{r}| \approx \alpha_0$, and the approximation (5) turns out to have no grounds.

In addition to the initial coordinate system, in which the atomic nucleus rests at the origin and the absolute value of the coordinate of the ground-state electron is of the order of $1/Z$ [Eqs. (1) and (6) are written in this system], the Kramers-Henneberger transformation introduces the new coordinate system. In the latter, the nucleus coordinates are given by $\boldsymbol{\alpha}(t)$ and, provided $\alpha_0 \gg 1/Z$, the absolute value of the coordinate of the ground-state electron is of the order of α_0 [Eqs. (3)–(5) and also (8) are given in the new system]. In the "derivation" of the Coulomb correction to the Volkov solution given in [1], there was a confusion of the space coordinates before and after the Kramers-Henneberger transformation. The approximation (5), which is the key ingredient of the consideration of [1], is the result of this confusion.

Although the results of [1] have been cited in quite a few articles, we were not able to find in the literature any critical discussion of the way these results were obtained. Moreover, there have even been attempts to "generalize" the "derivation" of [1] to the case of ionization of two-electron atoms (see [4]) and to "improve" its accuracy by taking (see [5,6])

$$V(|\mathbf{r}-\boldsymbol{\alpha}|) \approx -\frac{Z}{\alpha_0} - \frac{Z\boldsymbol{\alpha}\cdot\mathbf{r}}{\alpha_0^3}. \quad (8)$$

Since the region $r \approx \alpha_0$ in Eq. (3) is most important for the transition matrix element, clearly neither of the expansions (5) and (8) makes sense.

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