The role of excited discrete atomic states in the formation of quantum vortices in barrier-suppression ionization of hydrogen-like atom by ultrashort laser pulse

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Abstract. We theoretically examine the quantum vortices creating through barrier-suppression ionization of two dimensional hydrogen atom by ultrashort laser pulse. We show that for the considered case of ionization, the excited discrete atomic states do not impact on the vortex formation, and the problem can be considered in the single-level atom approximation.

1. Introduction

One of the interesting and actual aspects of atom ionization problem is to determine and to control the states of photoelectrons. A well-known example, when vortex photoelectrons are of interest not only from a fundamental point of view, but also have practical application perspectives, is photoemission spectroscopy with rescattering [1]. Another example is quantum vortices – the structures which are formed, in particular, by a photoelectron pulled out by a laser pulse with duration of the order of several atomic time units. These vortices are represented by specific regions in ordinary and momentum space, their centres correspond to the isolated zeros of the wave function, and the probability flux revolves around these centres. Due to the ultrashort interaction between the laser field and the atom, the photoelectron “remembers” its own initial bound state, and this circumstance can play an important role in the quantum vortices generation.

In our previews works [2-4], we considered, in particular, the barrier-suppression ionization of the two-dimensional (2D) hydrogen atom by an ultrashort laser pulse and investigated the formation of quantum vortices. The numerical investigation of this problem was based on the solution of the Schrödinger equation in the expanding space [5]. To obtain the analytical results, the standard nonstationary second order perturbation theory was used. We showed that the appearance of quantum vortices is due to the interference of the final photoelectron states with different orbital quantum numbers. One of the main approximations used in analytical consideration was neglecting of all excited states of atom (single-level atom approximation). In this paper, we generalize our analytical approach [4] and investigate the influence of atom excited states on the vortices formation. We also verify the applicability of the perturbation theory for a laser pulse with a relatively large amplitude $F_0 \approx 1$ (in atomic units).
2. Theoretical description of the vortex formation

In our work, we use the Hartree atomic system of units with \( h = m_e = e = 1 \), where \( h \) is the reduced Planck constant, \( m_e \) is the electron mass, and \( e \) is the elementary charge. We consider 2D-hydrogen atom \([6]\), which is affected by a laser pulse with time dependent amplitude \( \tilde{E}(t) = E(t)\tilde{e}_x \) polarized along \( x \) axis. The Hamiltonian of the system is

\[
\hat{H} = \hat{H}_0 + \hat{V}(t),
\]

where we use the polar coordinates \((\rho, \phi)\). Note that the nuclear charge is taken to be 1/2 \([2-4]\). The eigenstates of the unperturbed Hamiltonian \( \hat{H}_0 \) for the discrete energy spectrum are written as \( \Psi_{n,m}^{(0)} \equiv \psi_{n}^{(0)} \), where \( n = 1, 2, 3, \ldots \) and \( m = 0, \pm 1, \pm 2, \ldots, n-1 \) are the principal and orbital quantum numbers correspondingly. For a continuous energy spectrum, the wave functions are denoted as \( \Psi_{K_k}^{(0)} \equiv \psi_{K_k}^{(0)} \), where \( K = \sqrt{k_x^2 + k_y^2} \) and \( m = 0, \pm 1, \pm 2, \ldots \).

The Schrödinger equation in interaction picture has the form

\[
\left\{ i\frac{\partial}{\partial t} \Psi(t) \right\} = \hat{V}(t)\psi(t),
\]

where \( \hat{V}(t) \) is the interaction operator in interaction representation. Applying the standard nonstationary second order perturbation theory to equation (2), one can obtain the following expression for the probability amplitude \( b(\tilde{k}, t) \) that the photoelectron at moment \( t \) has the momentum \( \tilde{k} = (k_x, k_y) \)

\[
b(\tilde{k}, t) = b^{(1)}(\tilde{k}, t) + b^{(2)}(\tilde{k}, t) + b^{(2)}_{\mu\nu}(\tilde{k}, t),
\]

where

\[
\begin{align*}
b^{(1)}(\tilde{k}, t) &= (-i) \sum_{\tilde{k}', N_0} dt' V_{\tilde{k}', N_0}^{(1)}(t') \langle \tilde{k}' \psi_{\tilde{k}', N_0}^{(0)} \rangle, \\
b^{(2)}(\tilde{k}, t) &= (-i)^2 \sum_{\tilde{k}', \tilde{k}, N_0} dt' dt'' V_{\tilde{k}', \tilde{k}, N_0}^{(2)}(t', t'') \cdot V_{\tilde{k}', N_0}^{(1)}(t') \langle \tilde{k}' \psi_{\tilde{k}', N_0}^{(0)} \rangle, \\
b^{(2)}_{\mu\nu}(\tilde{k}, t) &= (-i)^2 \sum_{\tilde{k}', \tilde{k}, N} dt' dt'' V_{\tilde{k}', \tilde{k}, N}^{(2)}(t', t'') \cdot V_{\tilde{k}', N}^{(1)}(t') \langle \tilde{k}' \psi_{\tilde{k}', N}^{(0)} \rangle.
\end{align*}
\]

and \( V_{a,b}^{(1)}(t') = \langle a | \hat{V}(t') | b \rangle \) is the matrix elements of the interaction operator, the index \( N_0 \) corresponds to the initial ground state of an atom \( N_0 \rightarrow (n = 1, m = 0) \) with energy \( E_i = -0.5 \), and \( \langle \tilde{k} | \psi_{\tilde{k}, N}^{(0)} \rangle \) are the eigenstates of unperturbed Hamiltonian \( \hat{H}_0 \) in the momentum representation. In our previous works \([3,4]\), we took into account only two first terms in (3). The first \( b^{(1)}(\tilde{k}, t) \) and second \( b^{(2)}(\tilde{k}, t) \) terms in (3) describe, respectively, one-photon and two-photon transitions from initial state.
\[ |\Psi^{(0)}_{\mathcal{N}_k}\rangle \] into all possible states of the continuous spectrum \( |\Psi^{(0)}_{\mathcal{K}}\rangle \). The two-photon transition in the second term occurs through intermediate states of the continuous spectrum. The last (third) term \( b^{(2)}_{\text{db,kt}} \) in (3) also corresponds to the two-photon transition, but in this transition, the intermediate states relate to the discrete atomic states. To calculate this term, we will use the same approximation that we have already used in [3,4]. Namely, we replace eigenstates \( |\Psi^{(0)}_{\mathcal{K}}\rangle \) by cylindrical waves \( |\tilde{\Psi}^{(0)}_{\mathcal{K}}\rangle \), which have the following form in the position representation

\[
|\tilde{\Psi}^{(0)}_{\mathcal{K},m}\rangle = \tilde{R}_{\mathcal{K},m}(\rho)\Phi_m(\varphi) = J_{|m|}(k\rho)\frac{e^{\text{imp}}}{(2\pi)^{1/2}},
\]

where \( J_{|m|}(k\rho) \) is the Bessel function of the first kind. After some simple calculations, the third term can be written as

\[
b^{(2)}_{\text{db,kt}}(\tilde{k},t) = \left(-\frac{\text{i}}{2(2\pi)^{1/2}}\right)^2 \sum_{m,n=2}^{\infty} f_{k,n,1}(t) \left\{ \tilde{R}_{\mathcal{K},m}(\rho) |R_{n,m}\rangle \cos(2\varphi) \tilde{R}_{\mathcal{K},m}(\rho) |R_{n,m}\rangle \right\} |R_{n,m}\rangle |R_{n,m}\rangle,
\]

where

\[
f_{k,n,1}(t) = \int_0^\infty \int_0^\infty e^{\text{i}m\varphi} e^{\text{i}m\varphi} \tilde{E}(t') \cdot \tilde{E}(t^*),
\]

\( \tilde{k} = (k,\varphi) \) is the wave vector specified by its polar coordinates, \( \langle R_{m,n} | \rho | R_{n,m} \rangle \), \( \langle \tilde{R}_{\mathcal{K},m} | \rho | R_{n,m} \rangle \) are the radial components of the matrix elements of the transition dipole moment, where \( R_{n,m} \) corresponds to the radial part of the atom wave function \( \langle \tilde{\Psi}^{(0)}_{\mathcal{K},m} | \rho | \Phi_m(\varphi) \rangle \).

In the next section, we will check the influence of the third term (5) on the quantum vortex formation.

3. Results

We perform all calculations for the following time dependence of the field amplitude

\[
\tilde{E}(t) = F_0 \cos(\omega t) \left[ \theta(T - t) - \theta(-t) \right],
\]

where \( \theta(x) \) is the Heaviside step function, the pulse duration \( T = 4 \), the frequency \( \omega = \pi \) and the time-independent amplitude \( F_0 = 0.5; 1 \). The atom is initially in the ground state.

In figure 1a, we plot the square root of the probability density \( \rho \) for the photoelectron momentum when \( t >> T \), obtained numerically (for brevity, the words ‘square root’ is now omitted). Two vortices placed on the axis \( k_y \) symmetrically with respect to the origin are clearly visible. The zeros of probability are even better visible when comparing graphs for \( \rho(k_x,0,t >> T) \equiv \rho_x \) and \( \rho(0,k_y,t >> T) \equiv \rho_y \) (see figure 1b). The coordinates of pair of vortices are \( k_x \approx 0, k_y \approx \pm 2.3 \). As was shown in [2], the probability flux revolves around these zeros.
Figure 1. (a) Probability density $\rho$ for a photoelectron momentum for $t \gg T$. (b) Probability densities $\rho_x$ (black solid line) and $\rho_y$ (blue dash line) ($t \gg T$). Probabilities are normalized by the first left peak. The red circle indicates the center of the quantum vortex. Pulse parameters $F_0 = 0.5$, $T = 4$, $\omega = \pi$.

In figure 2, a, b, we compare numerical results presented in figure 1 with the analytical results obtained using expression (3). In the infinite sum by $n$ of the expression for $h_{d}^{(2)}(\vec{k}, t)$ (5), we take into account just first six $N_d = 6$ excited discrete atomic levels (the following enhancement of $N_d$ does not significantly affect the results). One can see that for given pulse parameters (regime of barrier-suppression ionization), the influence of the two-photon transitions through discrete atomic states on vortex formation is negligible, and the main changes occur for small values of wave vector magnitude. We should note that the high-quality prediction in the range of small $k$ is the well known problem not only for perturbation theory but also for numerical simulations [3].

In figure 2, c, d, we show the applicability of used perturbation theory for relatively large field amplitude $F_0 = 1$. As follows from figures, an increase in the field amplitude does not lead to a drastically worsening in the prediction quality. This can be explained by the fact that perturbation theory can be used in the case of sudden impact of a quantum system by a considerable not small perturbation [7].
Figure 2. Probability densities $\rho_x$ (a), (c) and $\rho_y$ (b), (d). Gray solid lines are the numerical simulations. Black dash lines and red dash-dot lines correspond to the analytical solution (3) without and with two-photon transitions through intermediate discrete atomic states correspondingly; (a) and (b) – laser amplitude $F_0 = 0.5$. (c) and (d) – larger laser amplitude $F_0 = 1$. Other pulse parameters $T = 4$, $\omega = \pi$. Probabilities are normalized by the first left peak.

4. Conclusion
In this paper, we considered the formation of quantum vortices in the case of barrier-suppression ionization of a two-dimensional hydrogen atom by an ultrashort laser pulse. We showed that for considered here and in our previews papers [2-4] laser field parameters $T \approx \omega \approx F_0 - 1$ the probability density for the photoelectron can be calculated in the second order perturbation theory without taken into account the two-photon electron transitions through intermediate states of atomic discrete spectrum.

We also considered the laser pulse with relatively large amplitude $F_0 = 1$ and showed that the analytical approach used can also describe an appearance of quantum vortices for such strong atom-field interaction. An explanation of the perturbation theory stability is the sudden on and off of the laser pulse.

Finally, we should note that such a vortex structure can be obtained using various types of ionization, using different quantum particles, and with different mechanisms of vortex formation. Thus, authors of [8] considered the ground-state positronium formation in positron-hydrogen collisions in the Ore gap. They showed that nature of vortices, which manifest itself in the scattering amplitude of positronium, induced by charge exchange.

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