

DOI: 10.18721/JPM.10409
УДК 530.145

FORMATION OF QUANTUM VORTICES UPON ATOM IONIZATION BY A PULSE OF ELECTROMAGNETIC WAVES

*S.Yu. Ovchinnikov¹, N.V. Larionov²,
A.A. Smirnovsky^{1,2}, A.A. Schmidt¹*

¹Ioffe Institute of the Russian Academy of Sciences, St. Petersburg, Russian Federation

²Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation

We investigate the space-time evolution of a photoelectron formed as a result of interaction of an ultrashort electromagnetic pulse with a hydrogen-like atom in the two-dimensional approximation. A characteristic feature of the considered evolution is the presence of singular points in the electron probability density, which can be interpreted as centers of quantum vortices. Based on numerical simulation of the time-dependent Schrödinger equation, we analyze localization, structure and number of quantum vortices in ordinary and momentum space. We have also considered the probability flux. We have established that the analyzed values given are strongly dependent on the duration of ultrashort electromagnetic pulse. The numerical solution is compared with the analytical one obtained in the framework of the Born approximation.

Keywords: quantum vortex; atom ionization; Schrödinger equation; numerical simulation; Born approximation

Citation: S.Yu. Ovchinnikov, N.V. Larionov, A.A. Smirnovsky, A.A. Schmidt, Formation of quantum vortices upon atom ionization by a pulse of electromagnetic waves, St. Petersburg Polytechnical State University Journal. Physics and Mathematics. 10 (4) (2017) 111–121 DOI: 10.18721/JPM.10409

ОБРАЗОВАНИЕ КВАНТОВЫХ ВИХРЕЙ ПРИ ИОНИЗАЦИИ АТОМА ИМПУЛЬСОМ ЭЛЕКТРОМАГНИТНОГО ПОЛЯ

*С.Ю. Овчинников¹, Н.В. Ларионов²,
А.А. Смирновский^{1,2}, А.А. Шмидт¹*

¹Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Российская Федерация

²Санкт-Петербургский политехнический университет Петра Великого, Санкт-Петербург, Российская Федерация

Проведено численное и аналитическое исследование пространственно-временной эволюции квантовой системы, образованной в результате взаимодействия электромагнитного поля с водородоподобным атомом в двумерном приближении. Характерной особенностью полученного решения является наличие особых точек (квантовых вихрей), анализ которых проведен путем введения плотности вероятности и плотности потока вероятности. Образующиеся в процессе ионизации вихри могут распространяться на макроскопические расстояния и проявляться в виде запрещенных областей в спектре волновых чисел. Для численного моделирования такой задачи используется специальное преобразование переменных — метод расширяющегося пространства. Проведен численный анализ зависимости количества квантовых вихрей и их положений от параметров электромагнитного импульса. Численное решение сравнивается с аналитическим, полученным в рамках борновского приближения.

Ключевые слова: квантовый вихрь; ионизация атома; уравнение Шрёдингера; численное моделирование; борновское приближение

Ссылка при цитировании: Овчинников С.Ю., Ларионов Н.В., Смирновский А.А., Шмидт А.А. Образование квантовых вихрей при ионизации атома импульсом электромагнитного поля // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2017. Т. 10. № 4. С. 111–123. DOI: 10.18721/JPM.10409

Introduction

Numerous studies have considered structures that can be interpreted as vortices in quantum systems [1–6]. For example, a vortex structure, generated by a focused laser beam in Bose–Einstein condensate, was discovered recently [1]. This structure is similar to the Kármán vortex street, well known in fluid dynamics [7].

There is reason to believe that similar structures may evolve in simple single-electron quantum systems. In particular, vortex-like formations were investigated for quantum systems produced through photoionization of a single atom [5] or through atom-ion collision [6]. These formations manifest themselves as specific regions in space (ordinary or momentum), with their own centers, which are forbidden regions for electrons (isolated zeros of a single-electron wave function), and probability flux revolving around these centers.

Understanding the nature of vortices and developing methods for controlling them is of clear interest for fundamental studies, as well as for solving applied problems, e.g., in photoelectron spectroscopy.

In this study, we investigate formation and evolution of quantum vortices on the example of the well-known problem of ionization of a hydrogen-like atom by a laser pulse. The existing approximate approaches to solving such problem (see, for example, [10, 11]) are usually inapplicable to analysis of the evolution of vortex structures. Thus, the solutions obtained using quasi-classical approaches do not include vortex structures as they are associated with singularities of quantum pressure discarded due to small \hbar^2 .

Nevertheless, this information can be obtained by means of numerical simulation of the nonstationary Schrödinger equation [4]. Besides, the hydrodynamic representation based on the Madelung equations [8] provides a clear interpretation for the solution to the problem on evolution of quantum vortices. Another benefit of this approach is that it allows to introduce quantum pressure [9] which (as noted above) governs vortex trajectories and can serve as an indicator of the evolution of the entire quantum system. However, the singularities appearing as probability density tends to zero make it problematic to use the Madelung equations for simulating evolution of these vortex-like structures, whose nature is similar to that of potential vortices considered in the theory of inviscid flow [7].

On the other hand, there are also some difficulties in numerically solving the nonstationary Schrödinger equation because the wave function of the photoelectron includes an oscillating factor taking the form

$$\exp\left(i\frac{m}{2\hbar}\frac{r^2}{t}\right)$$

(m and r are the mass and the position of the electron, t is the time), leading to divergence for large values of r and t .

This issue can be resolved, in particular, through removing strongly oscillating phases by transformation of variables in expanding space and by using time scaling [12, 13]. Notably, the evolving vortex structures can also propagate unchanged at macroscopic distances [4], where they can be detected experimentally.

This study introduces a hybrid approach to analysis of dynamics of quantum systems, comprising two stages:

numerical solution of the nonstationary Schrödinger equation in expanding space, which makes it possible to identify quantum vortex structures for large values of r and t ;

hydrodynamic interpretation including the distributions of such field quantities as probability density and probability current.

Based on this hybrid approach, we consider space-time evolution of the photoelectron generated due to ionization of a two-dimensional hydrogen-like atom by an ultrashort electromagnetic pulse.

The two-dimensional approximation is valid, in particular, if electron motion in an atom is confined to two degrees of freedom, for example, in case of motion in a semiconductor quantum well [14, 15]. Furthermore, such a simplified problem statement is well suited for testing the numerical algorithm and analyzing the evolution of vortex structures, since they are easy to identify in the two-dimensional case.

Additionally, we compare the data from numerical simulation with the analytical results obtaining within the framework of the first Born approximation.

Problem Statement

We consider the two-dimensional hydrogen-like atom interacting with an ultrashort electromagnetic pulse. The Hamiltonian for this problem is given by



$$\left\{ \begin{array}{l} \hat{H} = \hat{H}_0 + \hat{V}, \\ \hat{H}_0 = \frac{1}{2} \hat{p}^2 + U(\mathbf{r}) = \\ = -\frac{1}{2} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right) - \frac{1}{2\rho}, \\ \hat{V} = -\hat{\mathbf{d}} \tilde{\mathbf{E}}(t) = \rho \cos(\varphi) \tilde{E}(t), \end{array} \right. \quad (1)$$

where \hat{H}_0 is the Hamiltonian of a free atom; ρ and φ are the polar coordinates and for convenience we took the following potential

$$U = U_c/2,$$

where $U_c = -1/\rho$ is the ordinary Coulomb potential.

Interaction between an atom and electromagnetic field is described by the interaction part of the Hamiltonian \hat{V} , where $\hat{\mathbf{d}}$ is the atomic dipole moment operator, $\tilde{\mathbf{E}}(t) = \mathbf{e}_x \tilde{E}(t)$ is the electric field vector of an ultrashort pulse, polarized along the x axis, with the amplitude

$$\tilde{E}(t) = \begin{cases} E_0 \cos(\omega t), & 0 < t < T, \\ 0, & t > T, \end{cases} \quad (2)$$

where E_0 is the time-independent amplitude, ω is the frequency and T is the pulse duration.

Here we immediately formulated the Hamiltonian in atomic units $\hbar = 1$, $m_e = 1$, $e = 1$.

Numerical Method

We described the evolution of the given quantum system using an approach based on numerical solution of the non-stationary Schrödinger equation. The simulation program consists of several modules.

The first module is intended for numerically solving the Schrödinger equation in coordinate and momentum representations during interaction with the electromagnetic pulse. A standard algorithm calculating the propagator of the wave function (operator splitting method, see, for example, [16]) is used for the time increment:

$$\Psi(\mathbf{r}, t + \Delta t) = \exp(-i\hat{H}\Delta t) \Psi(\mathbf{r}, t). \quad (3)$$

This propagator is divided into three components depending, in the following manner, only on the coordinate operator and only on the momentum operator:

$$\begin{aligned} \Psi(\mathbf{r}, t + \Delta t) &= \exp\left(-i\frac{\hat{p}^2}{2} \frac{\Delta t}{2}\right) \times \\ &\times \exp\left[-i\left(U(\mathbf{r}) + \hat{V}\left(t + \frac{\Delta t}{2}\right)\right) \Delta t\right] \times \\ &\times \exp\left(-i\frac{\hat{p}^2}{2} \frac{\Delta t}{2}\right) \Psi(\mathbf{r}, t). \end{aligned} \quad (4)$$

The evolution of the wave function at half-steps $\Delta t/2$ is simulated in the momentum space; the wave function is converted to the momentum representation using the fast Fourier transform for this purpose. The central component of the propagator is calculated in the coordinate representation at step Δt using the inverse Fourier transform.

The second program module is intended for converting the wave function obtained after applying an external pulse, by transformation of variables in expanding (scaled) space, with the help of the variables introduced by Soloviev and Vinitsky [17]. This method is described in detail in [13]. Notably, the time $t \rightarrow \infty$ corresponds to scaled time $\tau \rightarrow -0$, and the Coulomb potential turns into a δ function. This makes it impossible to numerically calculate the equation up to $\tau = 0$; additionally, the calculation error increases near the origin.

We should also note that when $\tau \rightarrow -0$, the squared modulus of the transformed wave function is the probability density for the momentum of the photoelectron for $t \rightarrow \infty$, when field pulse has long ended (all bound states of the discrete spectrum collapse).

Since the space and momentum distribution of the photoelectron is the primary focus in our problem, the evolution of the quantum system was simulated in the calculations below up to the time $\tau = 0.001$ (in atomic units); it was found that the solution becomes virtually independent of scaled time τ .

Numerical Results

Numerical simulation of the evolution of the quantum system was carried out for the following parameters of the electromagnetic pulse (2): $E_0 = 0.5$, $\omega = \pi$, and pulse duration T varied in the integer range from 1 to 9. Thus, a pulse is either an even or an odd number of half-periods of oscillations.

It is assumed that the atom is initially in the ground state with the wave function (eigenwave function of Hamiltonian \hat{H}_0)

$$\Psi_{1,0}^{(0)}(\rho) = \sqrt{2/\pi} \exp(-\rho), \quad (5)$$

where the first subscript corresponds to the principal quantum number $n=1$ and the second subscript to projection of the orbital angular momentum along the z axis, $m=0$.

The nonstationary Schrödinger equation was solved numerically with the following parameters: the computational domain in the coordinate space was a 60×60 (a.u.)² square, covered with a uniform structured mesh of 2048×2048 cells; the time step was $\Delta t = 10^{-3}$ a.u. Such parameters were selected based on preliminary analysis of the accuracy of the solution to be obtained and grid convergence, providing acceptable quality of resolution of the wave function.

Let us first consider the case when pulse duration $T = 4$. Fig. 1, *a* plots the square root of probability density for the photoelectron (for brevity, the phrase ‘square root’ is omitted from now on)

$$|\Psi(x, y, T)| \equiv |\Psi|$$

on a logarithmic scale at the time when the pulse ends. Local regions with low values of $|\Psi|$ (white ‘spots’ in Fig. 1, *a*) are vortex structures.

Enlarged fragment of $|\Psi|$ together with vector plot of the probability current

$$\mathbf{J} = 1/2i(\Psi^* \nabla \Psi - \Psi \nabla \Psi^*)$$

are plotted in Fig. 1, *b* (for greater clarity, the vectors in the figure were filtered twice and their lengths are the same). Two vortices rotating in opposite directions can be observed in this region. Another vortex structure is lo-

cated farther from the center but has worse resolution due to extremely small $|\Psi|$ values in this region. Other vortex structures that cannot be resolved on this mesh may be present. All of these structures can be born, and then move and annihilate each other over time. Fig. 1, *b* shows the precise moment when a vortex pair is born.

Since we are primarily interested in the vortex structures moving away from the center of the system ‘at infinity’ and manifesting for continuous spectrum, we are going to consider the probability density for $t \gg T$ obtained using the expanding space method with $\tau \rightarrow -0$. We are then going to plot the probability density for the momentum of the photoelectron

$$|\Psi(k_x, k_y, t \rightarrow \infty)| \equiv |b|$$

Fig. 2, *a* plots the probability density for the momentum with $t \gg T$ (on a logarithmic scale). Two vortices located on the axis k_y symmetrically with respect to the origin are clearly visible; an enlarged fragment with the vector plot of probability current in momentum representation is shown in Fig. 2, *b*. Thus, a pair of symmetric vortices evolves due to ionization of an atom by an electromagnetic pulse. A saddle point can be seen at $k_x = -0.4$, $k_y = 2.2$.

Let us now consider the probability density for momentum with smaller T . Fig. 3 plots the probability $|b|$ for $T = 1$ and $T = 2$. There are apparently no vortex structures at $T = 1$ (possibly due to insufficient grid resolution), while probability density turns out to be strongly asymmetric at small values of k_x (see Fig. 3, *a*).

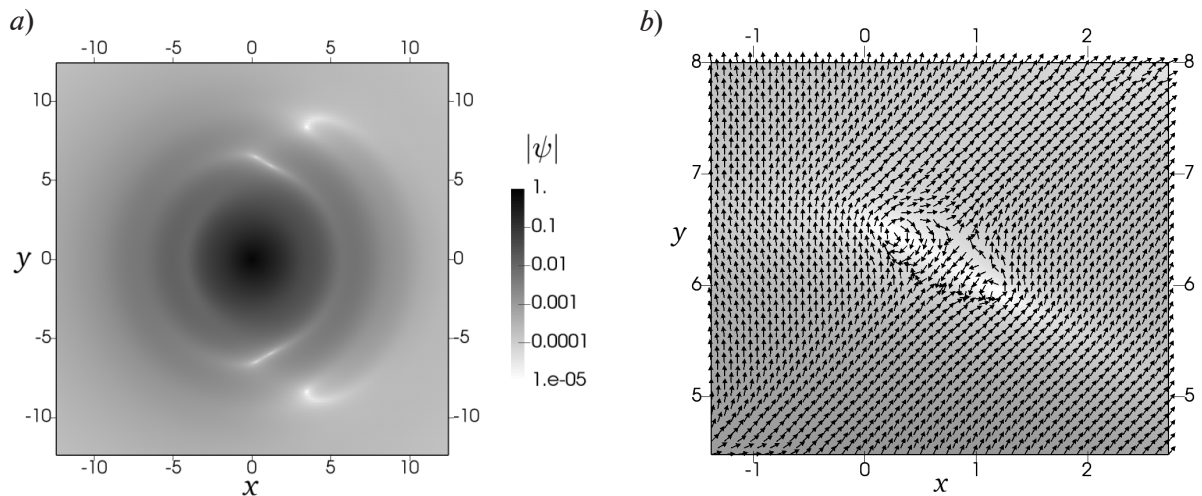


Fig. 1. Probability density of photoelectron, $|\Psi(x, y, T)| \equiv |\Psi|$, at pulse end (*a*) and its enlarged fragment with vector plot of probability current near vortex structure (*b*); birth of vortex pair is shown; $T = 4$

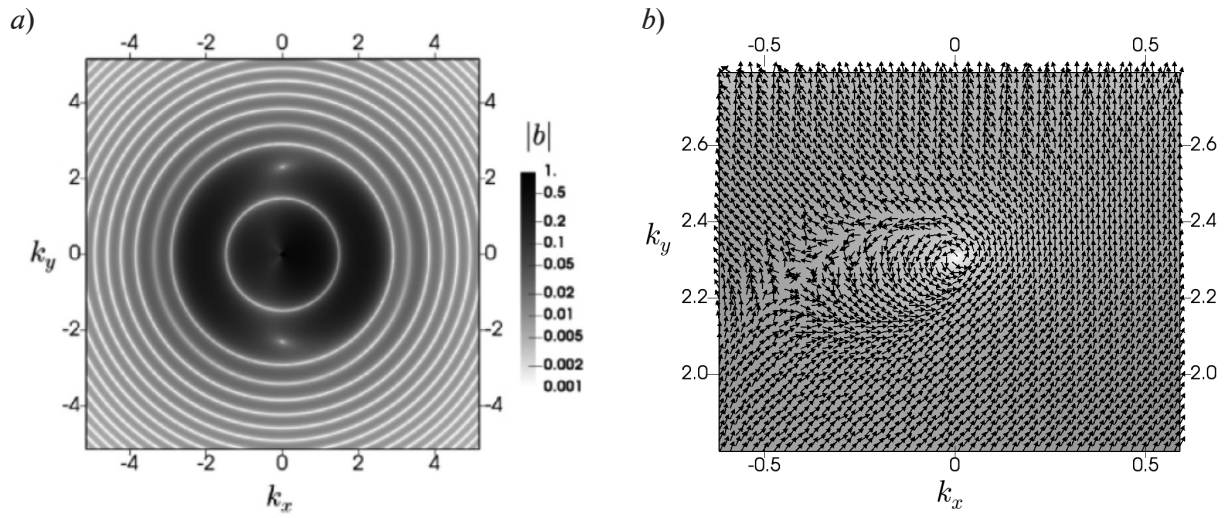


Fig. 2. Probability density for momentum of photoelectron for $t \gg T$, $|\Psi(k_x, k_y, t \rightarrow \infty)| \equiv |b|$ (a) and vector plot of probability current in momentum representation near quantum vortex (b); $T = 4$

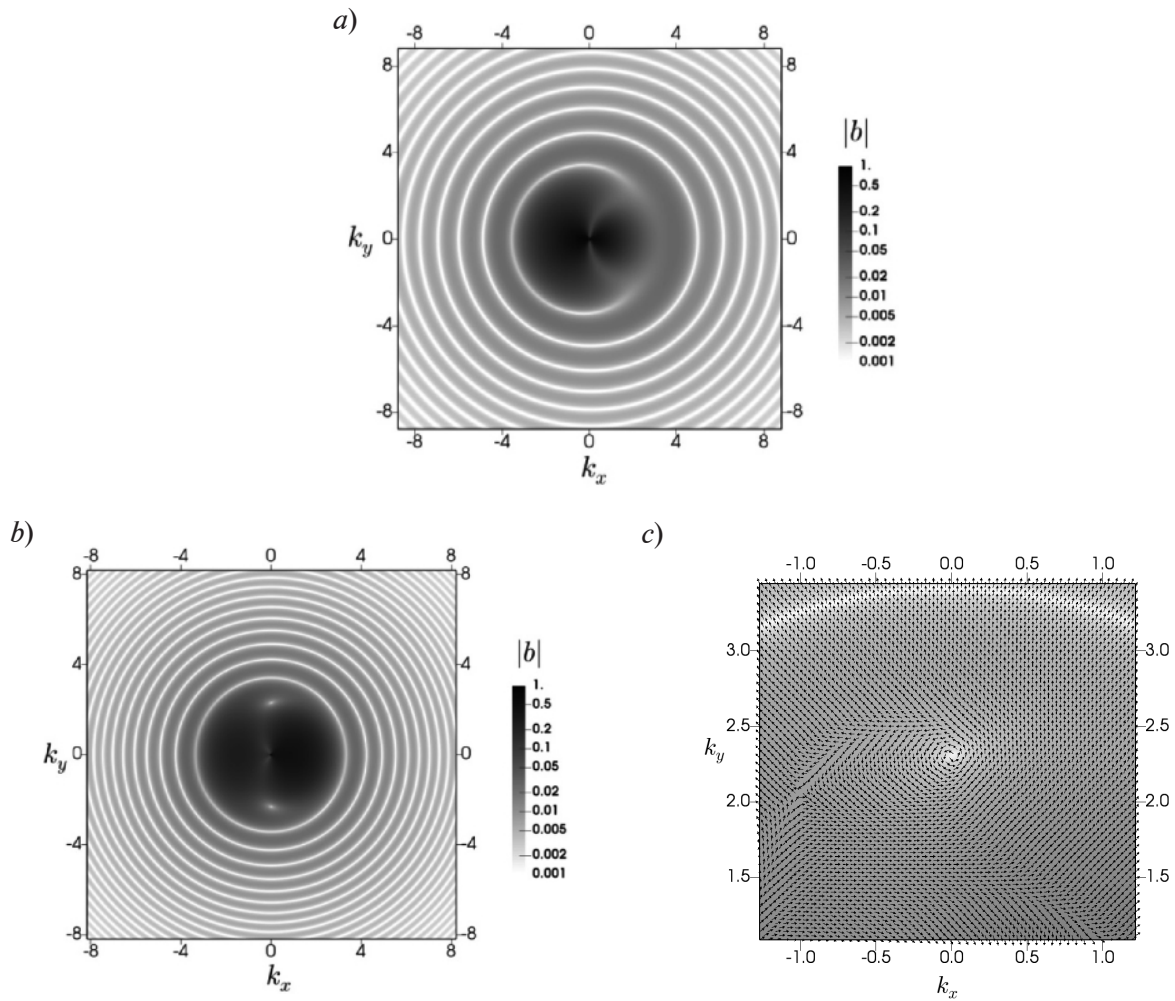


Fig. 3. Probability density for momentum of photoelectron for $t \gg T$, $|\Psi(k_x, k_y, t \rightarrow \infty)| \equiv |b|$, for different pulse durations T : $T = 1$ (a), no quantum vortices observed; $T = 2$ (b) and enlarged fragment with vector plot of probability current near quantum vortex (c)

As seen from Fig. 3, *b*, a pair of pronounced symmetric vortices evolve with increased pulse duration ($T = 2$); their position corresponds to the position of vortices at $T = 4$ to a high degree of accuracy. An enlarged fragment with the vector plot of probability current near the vortex is shown in Fig. 3, *c*. Apparently, the vortex is resolved on the mesh with good accuracy.

Evidently, a pair of vortices evolve in the same region with the coordinates $k_x \approx 0$, $k_y \approx \pm 2.3$ if the number of pulse half-periods is even ($T = 2, 4, 6, 8$). No other distinct vortices can be observed in this case.

The opposite situation occurs with an odd number of pulse half-periods ($T = 3, 5, 7, 9$). The position of the distinct vortex changes with changing T . Fig. 4 plots the probability density $|b|$ and probability current for pulse duration $T = 3$ as an example. Several vortex structures evolve but only the pair closer to the origin is best resolved. Notably, the coordinates of the vortex position approach the origin with increasing T .

Fig. 5 plots the probability density for fixed zero $k_y = 0$

$$|\Psi(k_x, k_y = 0, t \rightarrow \infty)| \equiv |b(k_x)|$$

for several values of T . A narrow peak starts to form as T increases, corresponding to the situation for ionization by monochromatic field at $T \rightarrow \infty$ and centered on the value

$$k_x = \pm \sqrt{2(\omega + E_1)} \approx \pm 2.3$$

where $E_1 = -0.5$ is the energy of the ground state of the hydrogen atom.

The probability $|b(k_x)|$ exhibits a clear asymmetry of the peaks centered close to $k_x \approx \pm 2.3$ with respect to the origin, while the heights of these peaks are almost identical for even duration $T = 8$. Another consideration is that due to the specifics of calculations in expanding space (in particular, because the Coulomb potential tends to the δ function), numerical simulation yields oscillations and a sharp increase in $|b(k_x)|$ with $k_x \rightarrow 0$.

First-order Born Approximation

Numerical simulation based on the nonstationary Schrödinger equation includes the entire spectrum of processes describing the evolution of the given quantum system but does not necessarily explain the physical mechanisms of the phenomena considered. For this reason, it is of particular interest to find approximate analytical solutions to the problem, allowing to obtain a clear physical interpretation of the process. We estimated the applicability of the first-order Born approximation to solving the given problem.

We can represent the solution of the nonstationary Schrödinger equation as an expansion in eigenwave functions $\Psi^{(0)}$ of an unperturbed Hamiltonian [14]:

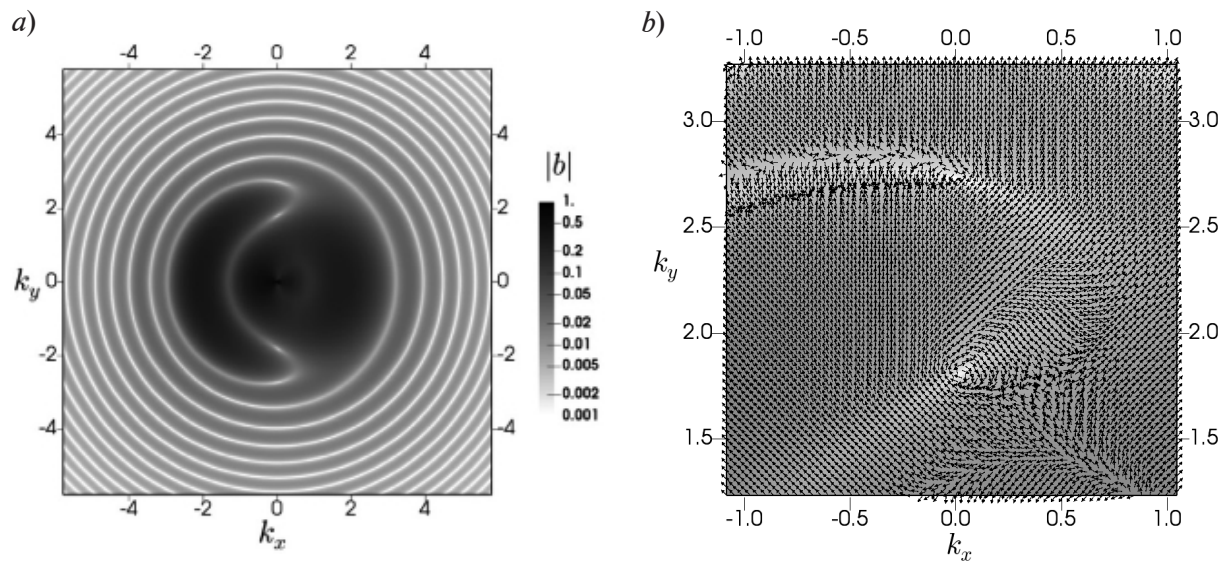


Fig. 4. Probability density for momentum of photoelectron for $t \gg T$, $|\Psi(k_x, k_y, t \rightarrow \infty)| \equiv |b|$ (a) and fragment with vector plot of probability current near two quantum vortices (b); $T = 3$

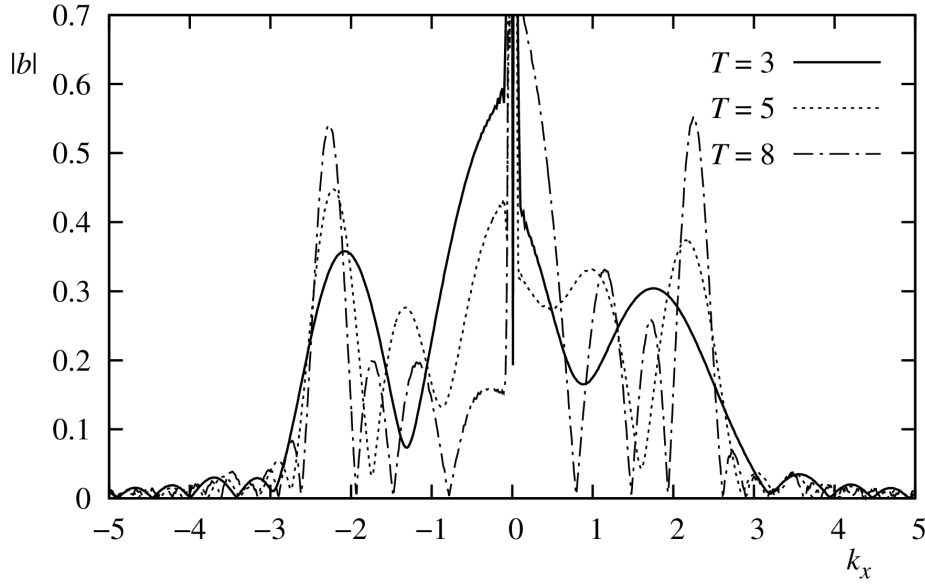


Fig. 5. Probability density for momentum of photoelectron for $t \gg T$, $|\Psi(k_x, k_y = 0, t \rightarrow \infty)| \equiv |b(k_x)|$, for different pulse durations

$$\Psi(\mathbf{r}, t) = \sum_{n,m} a_{n,m}(t) e^{-iE_n t} \Psi_{n,m}^{(0)}(\mathbf{r}) + \sum_m \int_0^\infty b_{E,m}(t) e^{-iEt} \Psi_{E,m}^{(0)}(\mathbf{r}) dE, \quad (5)$$

where $\Psi_{n,m}^{(0)}$ is the wave function of the discrete spectrum; $n = 1, 2, \dots$ is the principal quantum number; $m = 0, \pm 1, \pm 2, \dots, \pm(n-1)$ is the magnetic quantum number; the discrete spectrum energy is:

$$E_n = -\frac{1}{8(n-1/2)^2};$$

$\Psi_{E,m}^{(0)}$ is the wave function of the continuous spectrum (Coulomb wave) and the corresponding energy

$$E = k^2 / 2 = E_x + E_y = (k_x^2 + k_y^2) / 2$$

$$m = 0, \pm 1, \pm 2 \dots$$

Expanding the amplitudes $a(t)$ and $b(t)$ as a series in powers of small perturbations and leaving only the terms up to and including the first order, we obtain:

$$\begin{aligned} \Psi(\mathbf{r}, t) &= \Psi^{(0)}(\mathbf{r}, t) + \Psi_d^{(1)}(\mathbf{r}, t) + \Psi_c^{(1)}(\mathbf{r}, t) = \\ &= e^{-iE_1 t} \Psi_{1,0}^{(0)}(\mathbf{r}) + \sum_{n,m} a_{n,m;1,0}^{(1)}(t) e^{-iE_n t} \Psi_{n,m}^{(0)}(\mathbf{r}) + \\ &+ \sum_m \int_0^\infty b_{E,m;1,0}^{(1)}(t) e^{-iEt} \Psi_{E,m}^{(0)}(\mathbf{r}) dE, \end{aligned} \quad (6)$$

where it is assumed that the atom is in the ground state at the initial time (denoted by additional subscripts (1,0)); the superscripts for wave functions and amplitudes correspond to the order of smallness. The function $\Psi_d^{(1)}$ corresponds to transition to the excited state of the discrete spectrum (the second term in Eq. (6)), and $\Psi_c^{(1)}$ to transition to the excited state of the continuous spectrum (the last term in Eq. (6)).

We shall consider the following probability densities for momentum of photoelectron $|\Psi(k_x, k_y=0, t)| \equiv |b(k_x, t)|$ and $|\Psi(k_x=0, k_y, t)| \equiv |b(k_y, t)|$. To find them, let us write $\Psi_c^{(1)}$ in k_x and k_y representations, replacing the Coulomb wave under the integral with a cylindrical wave

$$\tilde{\Psi}_{E,m}^{(0)}(\mathbf{r}) = J_{|m|}(\sqrt{2E}\rho) \exp(im\varphi) / \sqrt{2\pi}$$

(wave function of the free electron).

In the first order of perturbation, we obtain the following expressions for $b(k_x, t)$ and $b(k_y, t)$:

$$\begin{cases} b^{(1)}(k_x, t) = e^{iE_x t} \langle k_x | \Psi_c^{(1)}(t) \rangle = \\ = \sum_m [i \cdot \text{sgn}(k_x)]^{-|m|} b_{E_x, m; 1, 0}^{(1)}(t), \\ b^{(1)}(k_y, t) = e^{iE_y t} \langle k_y | \Psi_c^{(1)}(t) \rangle = \\ = \sum_m [\pm \text{sgn}(k_y)]^{-|m|} b_{E_y, m; 1, 0}^{(1)}(t), \end{cases} \quad (7)$$

where the plus sign for $b^{(1)}(k_y, t)$ corresponds to the case $m > 0$, the minus sign corresponds to the case $m < 0$. The expressions after the first equality in (7) are the scalar product of the states $|\Psi^{(1)}(t)\rangle$ and $|k_i\rangle$ ($i=x, y$) in the bra-ket notation. The ket $|k_x\rangle$ corresponds to the state of a particle with a certain momentum and takes the form

$$\langle x|k_x\rangle \equiv \varphi_{k_x}(x) = \exp(ik_x x) / \sqrt{2\pi}$$

in the coordinate representation (the situation is similar for the ket $|k_y\rangle$).

We obtained probabilities (7) using the following properties and representations of Bessel functions:

$$\int_0^\infty J_m(k\rho) J_m(k'\rho) \rho d\rho = \delta(k-k') / k,$$

$$J_m(x) = (i^m / 2\pi) \int_0^{2\pi} \exp(-ix \cos \varphi + im\varphi) d\varphi, \quad (8)$$

$$J_m(x) = (1 / 2\pi) \int_0^{2\pi} \exp(-ix \sin \varphi + im\varphi) d\varphi.$$

To find $b_{E,m}^{(1)}(t)$, let us substitute expansion (6) into the Schrödinger equation; we obtain the following expression:

$$\begin{aligned} b_{E,m}^{(1)}(t) &= -i \int_0^t \langle \tilde{\Psi}_{E,m}^{(0)} | \hat{V} | \Psi_{1,0}^{(0)} \rangle dt' = \\ &= i(\delta_{m,1} + \delta_{m,-1}) \cdot \frac{3\sqrt{2E}}{(1+2E)^{5/2}} \int_0^t \tilde{E}(t') e^{i\omega_{E1}t'} dt', \end{aligned} \quad (9)$$

where $\omega_{E1} = E - E_1$.

At last, $b^{(1)}(k_x, t)$ and $b^{(1)}(k_y, t)$ take the following final form:

$$\begin{cases} b^{(1)}(k_x, t) = \frac{6|k_x|}{(1+k_x^2)^{5/2}} \\ \times \int_0^t \tilde{E}(t') e^{i\omega_{E1}t'} dt', \\ b^{(1)}(k_y, t) = 0. \end{cases} \quad (10)$$

Fig. 6 compares analytical result (10) with the result of numerical simulation for the pulse $\tilde{E}(t)$ defined by Eq. (2).

Let us discuss some of the peculiarities observed. The numerical result and the analytical solution diverge greatly in the region of small wave numbers ($k_x \approx 0$). This is due to several factors:

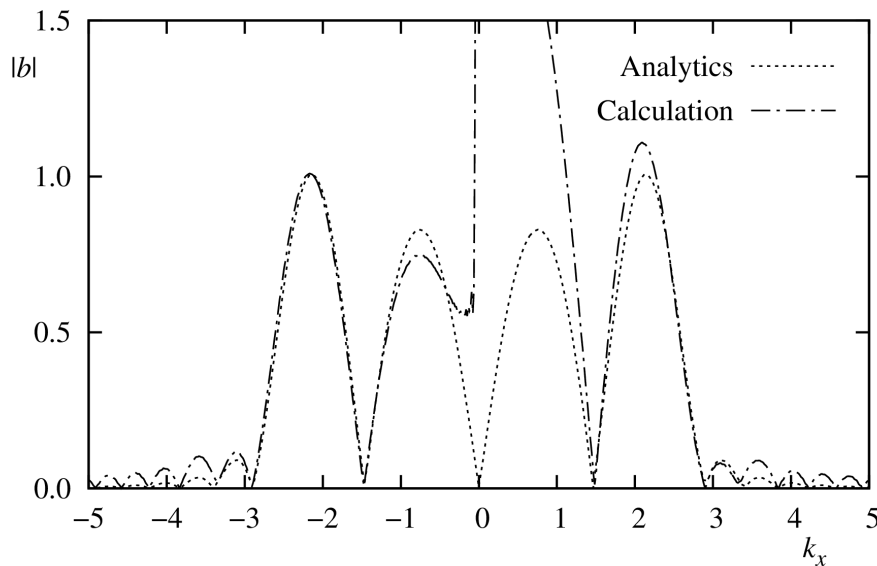


Fig. 6. Comparison of analytical calculation and numerical simulations (probabilities are normalized to left resonance peak); $T = 4$



large ‘error’ in numerical simulation in this region because of the above-mentioned specifics of calculations in scaled space, which does not allow to regard the result obtained for small k_x as close to true;

well-known limitations of the Born approximation, implying, in our case, that the Coulomb wave in (5) is replaced by a cylindrical wave.

However, the agreement between numerical simulation and analytical solution in the region of resonance values

$$k_x \approx \pm \sqrt{2(\omega + E_1)}$$

is rather good, even though the Born approximation does not describe the asymmetry of the distribution with respect to $k_x = 0$. This asymmetry is fairly natural (see also Fig. 1), since the evolution of the wave function of the electron in an initially bound state absolutely cannot have the same symmetry, despite the ‘symmetric’ effect of the electric pulse in time.

The vortices that could be identified for the given pulse duration by analyzing the probability $|b(k_y, t)|$ are not described by the first-order Born approximation, since $b^{(1)}(k_y, t) = 0$ (see Eq. (10)).

Thus, it seems natural to assume that the second order of perturbation theory, containing transitions through intermediate states, should allow to identify vortices most likely associated with destructive interference of such transitions.

Conclusion

Based on numerical simulation of the nonstationary Schrödinger equation, we have carried out studies on space-time evolution of a photoelectron appearing due to interaction of an ionizing electromagnetic ultrashort pulse with a hydrogen-like atom in the two-dimensional approximation. We have shown that vortex-

like structures appeared during atom-field interaction: the probability density of the photoelectron has isolated zeros in the centers of these vortices, and the corresponding probability fluxes revolve around each these centers. The evolution of vortices in time is associated with their annihilation, birth and modifications. Finally, there are only stable vortices remaining with $t \rightarrow \infty$, and they can be observed at long distances from the parent atom.

We have shown that localization of the vortices strongly depends on pulse duration T . Thus, the positions of vortices in momentum space for the given cosine pulse with fixed parameters $E_0 = 0.5$ and $\omega = \pi$ remained the same with different T , which was equal to an even number of half-periods ($T = 2, 4, 6, 8$). If the duration T was equal to an odd number of half-periods ($T = 3, 5, 7, 9$), the centers of the vortices shifted towards the origin as T increased and new vortex structures formed. There were no vortices when pulse duration was $T = 1$.

We have obtained analytical expressions for probability density for the momentum of the photoelectron within the first-order Born approximation. Quantum vortices could not be identified by these expressions, indicating that quantum vortices are generated by destructive interference of transitions through different intermediate states of discrete or continuous spectra, which can be taken into account in the second order of perturbation theory.

We expect to carry out more detailed studies of this problem in a separate paper by constructing perturbation theory series.

The information obtained in our work may be useful in design of experimental studies on related problems.

The study was financed by RFBR, grant no. 15-02-07794.

REFERENCES

- [1] **R.M. Wilson**, An obstacle dragged through a Bose–Einstein condensate can leave a well-known pattern of vortices in its wake, *Physics Today*. 70 (1) (2017) 19, <http://dx.doi.org/10.1063/PT.3.3416>
- [2] **G. Krstulovic, N. Brachet, E. Tirapogui**, Radiation and vortex dynamics in the nonlinear Schrödinger equation, *Phys. Rev. E*. 78 (2) (2008) 026601.
- [3] **J.M. NgokoDjiokap, A.V. Meremianin, et al.**, Multistart spiral electron vortices in ionization by circularly polarized UV pulses, *Phys. Rev. A*. 94 (1) (2016) 013408.
- [4] **S.Y. Ovchinnikov, J.H. Macek, D.R. Schultz**, Hydrodynamical interpretation of angular momentum and energy transfer in atomic processes, *Phys. Rev. A*. 90 (6) (2014) 062713.
- [5] **J.M. NgokoDjiokap, S.X. Hu, L.B. Madsen, et al.**, Electron vortices in photoionization by circularly polarized attosecond pulses, *Phys. Rev. Lett.* 115 (11) (2015) 113004.
- [6] **L.Ph.H. Schmidt, C. Goihl, D. Metz, et al.**, Vortices associated with the wavefunction of a single electron emitted in slow ion-atom collisions, *Phys. Rev. Lett.* 112 (8) (2014) 083201.

- [7] **L.G. Loitsyanskiy**, Mechanics of liquids and gases, New York, Begell House, 1995.
- [8] **E. Madelung**, Quantentheorie in Hydrodynamischer Form, Z. Physik. 40 (1926) 332–326.
- [9] **T. Takabayasi**, On the formulation of quantum mechanics associated with classical pictures, Prog. Theor. Phys. 8 (2) (1952) 143–182.
- [10] **M.V. Fedorov**, L.V. Keldysh's "Ionization in the field of a strong electromagnetic wave" and modern physics of interaction of atoms with a strong laser field, JETP. 2016, 122 (3) (2016) 449–455.
- [11] **N.B. Delone, V.P. Krainev**, Nelineynaya ionizatsiya atomov lazernym izlucheniem [Nonlinear ionization of atoms by laser radiation], Moscow, Physmatlit, 2001.
- [12] **S.Yu. Ovchinnikov, G.N. Ogurtsov, J.H. Macek, Yu.S. Gordeev**, Dynamics of ionization in atomic collisions, Phys. Rep. 389 (3) (2004) 119–159.
- [13] **S.Yu. Ovchinnikov, A.A. Smirnovsky, A.A. Schmidt**, Development of an algorithm of hydrodynamic analysis of quantum system evolution in expanding space, Tech. Phys. Lett. 42 (4) (2016) 407–410.
- [14] **X.L. Yang, S.H. Guo, F.T. Chan, et al.**, Analytic solution of a two-dimensional hydrogen atom. I. Nonrelativistic theory, Phys. Rev. A. 43 (3) (1991) 1186–1196.
- [15] **D.G.W. Parfitt, M.E. Portnoi**, The two-dimensional hydrogen atom revisited, Journal of Mathematical Physics. 43 (10) (2002) 4681–4691.
- [16] **A.D. Bandrauk, H. Shen**, Higher order exponential split operator method for solving time-dependent Schrödinger equations, Canadian Journal of Chemistry. 70 (2) (1992) 555–559.
- [17] **E.A. Soloviev, S.I. Vinitzky**, Suitable coordinates for the three-body problem in the adiabatic representation, Journal of Physics. B. 18 (16) (1985) L557–L562.

Received 21.09.2017, accepted 18.10.2017.

THE AUTHORS

OVCHINNIKOV Sergey Yu.

Ioffe Institute of the Russian Academy of Sciences

26 Polytekhnicheskaya St., St. Petersburg, 194021, Russian Federation
sovichin@utk.edu

LARIONOV Nikolay V.

Peter the Great St. Petersburg Polytechnic University

29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation
larionov.nickolay@gmail.com

SMIRNOVSKY Alexander A.

Peter the Great St. Petersburg Polytechnic University

29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation smirta@mail.ru

SCHMIDT Alexander A.

Ioffe Institute of the Russian Academy of Sciences

26 Polytekhnicheskaya St., St. Petersburg, 194021, Russian Federation
alexander.schmidt@mail.ioffe.ru

СПИСОК ЛИТЕРАТУРЫ

1. **Wilson R.M.** An obstacle dragged through a Bose–Einstein condensate can leave a well-known pattern of vortices in its wake // Physics Today. 2017. Vol. 70. No. 1. P. 19. <http://dx.doi.org/10.1063/PT.3.3416>
2. **Krstulovic G., Brachet N., Tirapegui E.** Radiation and vortex dynamics in the nonlinear Schrödinger equation // Phys. Rev. E. 2008. Vol. 78. No. 2. P. 026601.
3. **Ngoko Djiokap J.M., Meremianin A.V., Manakov N.L., Hu S.X., Madsen L.B., Starace A.F.** Multistart spiral electron vortices in ionization by circularly polarized UV pulses // Phys. Rev. A. 2016. Vol. 94. No. 1. P. 013408.
4. **Ovchinnikov S.Y., Macek J.H., Schultz D.R.** Hydrodynamical interpretation of angular momentum and energy transfer in atomic processes // Phys. Rev. A. 2014. Vol. 90. No. 6. P. 062713.
5. **Ngoko Djiokap J.M., Hu S.X., Madsen L.B., Manakov N.L., Meremianin A.V., Starace**



- A.F. Electron vortices in photoionization by circularly polarized attosecond pulses // Phys. Rev. Lett. 2015. Vol. 115. No. 11. P. 113004.
6. Schmidt L.Ph.H., Goihl C., Metz D., Schmidt-Böcking H., Dürner R., Ovchinnikov S.Yu., Macek J.H., Schultz D.R. Vortices associated with the wavefunction of a single electron emitted in slow ion-atom collisions // Phys. Rev. Lett. 2014. Vol. 112. No. 8. P. 083201.
7. Лойцянский Л.Г. Механика жидкости и газа. М.: Дрофа, 2003. 600 с.
8. Madelung E. Quantentheorie in Hydrodynamischer Form // Z. Physik. 1926. Vol. 40. Pp. 332–326.
9. Takabayashi T. On the formulation of quantum mechanics associated with classical pictures // Prog. Theor. Phys. 1952. Vol. 8. No. 2. Pp. 143–182.
10. Федоров М.В. Работа Л.В. Келдыша «Ионизация в поле сильной электромагнитной волны» и современная физика взаимодействия атомов с сильным лазерным полем // ЖЭТФ. 2016. Т. 149. Вып. 3. С. 522–529.
11. Делоне Н.Б., Крайнев В.П. Нелинейная ионизация атомов лазерным излучением. М.: Физматлит, 2001. 320 с.
12. Ovchinnikov S.Yu., Ogurtsov G.N., Macek J.H., Gordeev Yu.S. Dynamics of ionization in atomic collisions // Phys. Rep. 2004. Vol. 389. No. 3. Pp. 119–159.
13. Овчинников С.Ю., Смирновский А.А., Шмидт А.А. Разработка алгоритма гидродинамического анализа эволюции квантовых систем в расширяющемся пространстве // Письма в ЖТФ. 2016. Т. 42. № 8. С. 37–44.
14. Yang X.L., S.H. Guo, F.T. Chan, K.W. Wong, W.Y. Ching. Analytic solution of a two-dimensional hydrogen atom. I. Nonrelativistic theory // Phys. Rev. A. 1991. Vol. 43. No. 3. Pp. 1186–1196.
15. Parfitt D.G.W., Portnoi M.E. The two-dimensional hydrogen atom revisited // Journal of Mathematical Physics. 2002. Vol. 43. No. 10. Pp. 4681–4691.
16. Bandrauk A.D., Shen H. Higher order exponential split operator method for solving time-dependent Schrödinger equations // Canadian Journal of Chemistry. 1992. Vol. 70. No. 2. Pp. 555–559.
17. Soloviev E.A., Vinitzky S.I. Suitable coordinates for the three-body problem in the adiabatic representation // Journal of Physics. B. 1985. Vol. 18. No. 16. Pp. L557–L562.

Статья поступила в редакцию 21.09.2017, принята к публикации 18.10.2017.

СВЕДЕНИЯ ОБ АВТОРАХ

ОВЧИННИКОВ Сергей Юрьевич — доктор физико-математических наук, старший научный сотрудник Физико-технического института им. А.Ф. Иоффе РАН.
194021, г. Санкт-Петербург, Политехническая ул., 26
sovichin@utk.edu

ЛАРИОНОВ Николай Владимирович — кандидат физико-математических наук, научный сотрудник Санкт-Петербургского политехнического университета Петра Великого.
195251, Россия, г. Санкт-Петербург, Политехническая ул., 29
larionov.nickolay@gmail.com

СМИРНОВСКИЙ Александр Андреевич — кандидат физико-математических наук, доцент Санкт-Петербургского политехнического университета Петра Великого.
195251, Россия, г. Санкт-Петербург, Политехническая ул., 29
smirta@mail.ru

ШМИДТ Александр Александрович — кандидат физико-математических наук, заведующий сектором Физико-технического института им. А.Ф. Иоффе РАН.
194021, Санкт-Петербург, Политехническая ул., 26
alexander.schmidt@mail.ioffe.ru