

The wave function of a photoelectron near the center of a quantum vortex

© N.V. Larionov^{1,2}, Yu.L. Kolesnikov¹, V.M. Molchanovskiy¹

¹ State Marine Technical University, St. Petersburg, Russia

² Peter the Great Saint-Petersburg Polytechnic University, St. Petersburg, Russia

e-mail: larionov.nickolay@gmail.com

Received March 13, 2024

Revised May 28, 2024

Accepted May 28, 2024

The behavior of a photoelectron in the vicinity of the localization of the quantum vortex is theoretically investigated in a two-dimensional approximation. The obtained photoelectron wave function has a simple structure, which is the product of a Gaussian wave packet by a polynomial containing information about the vortex. With its help, the probability density and current are analyzed, both in momentum and coordinate spaces. The effect of the intensity of an ionizing ultrashort laser pulse on the shape of a quantum vortex is also investigated.

Keywords: photoelectron, quantum vortex, momentum representation, probability flux, ultrashort pulse.

DOI: 10.61011/EOS.2024.05.59114.6140-24

1. Introduction

In our previous studies we have investigated quantum vortices forming during the over-barrier ionization of a two-dimensional hydrogen atom by an ultrashort laser pulse [1–4]. The calculations were conducted using both a numerical solution of the Schrödinger equation and analytical approach based on the non-stationary perturbation theory. In the latter case, a analytical expression has been obtained for a photoelectron function in the momentum k -representation. This wave function was used to identify the quantum vortex centers and to analyze the „symmetric“ flow of probability [5] in the corresponding k -space.

Transition from the k -space to the conventional coordinate space has not been performed for the obtained wave function. The reason behind this are significant difficulties in the two-dimensional Fourier transform.

In this work, for the case of well localized vortices, we can successfully simplify the above-mentioned photoelectron wave function so that it is written as a product of the Gaussian function of the momentum modulus $k = |\mathbf{k}|$ and the polynomial with respect to the projections k_x, k_y . Such simplified wave function does not lose any information about a quantum vortex and allows a quantum vortex to be easily examined in the coordinate space.

For the purpose of this study, a system of atomic units ($\hbar = 1, m_e = 1, e = 1$) is used, where the atomic unit of electric field F_a is equal to the Coulomb field strength at the Bohr radius, and the atomic unit of time T_a multiplied by 2π is the orbital period of an electron in the same Bohr model.

2. Theoretical model

The given model is represented by a two-dimensional hydrogen atom [6] exposed to an ultrashort laser pulse. The

„atom+field“ interaction operator is written in the dipole approximation:

$$\hat{V} = -\hat{\mathbf{d}}\mathbf{F}(t), \quad (1)$$

where $\hat{\mathbf{d}} = -\hat{\mathbf{r}} = -(\mathbf{e}_x\hat{x} + \mathbf{e}_y\hat{y})$ is the atomic dipole moment operator and $\mathbf{e}_x, \mathbf{e}_y$ are the unit vectors of the Cartesian coordinate system. The electric field strength vector of laser $\mathbf{F}(t)$ is simulated by the following function:

$$\mathbf{F}(t) = (F_x(t), 0) = \mathbf{e}_x F_0 \cos(\omega t - \alpha) [\theta(T - t) - \theta(-t)], \quad (2)$$

where ω is the frequency, $\theta(t)$ is the Heaviside function, T is the pulse duration, α is the initial phase. The constant amplitude F_0 values are taken such that the over-barrier ionization predominates.

The electron wave function is sought as a sum of the ground (initial) state of the atom and a state corresponding to the continuous spectrum [7]. The latter is written as a superposition of cylindrical waves with unknown amplitudes that are in turn calculated using the non-stationary perturbation theory.

Omitting the intermediate calculations that have been described in detail in our previous works, we write a part of the wave function in the momentum representation responsible for the continuous spectrum of the electron (hereinafter referred to as the photoelectron):

$$\tilde{\Psi}(k, \varphi_k, t) = \sum_m b_{k,m}(t) (-i)^{|m|} \Phi_m(\varphi_k) e^{-iE_k t}. \quad (3)$$

Here, (k, φ_k) are polar momentum components \mathbf{k} of the photoelectron, $m = 0, \pm 1, \pm 2, \dots$ is the photoelectron angular momentum projection on the z axis and $E_k = k^2/2 = (k_x^2 + k_y^2)/2$ is the photoelectron energy. $\Phi_m(\varphi_k) = e^{im\varphi_k}/\sqrt{2\pi}$ is the angular part of the wave function.

Amplitudes $b_{k,m}(t)$ satisfy the following system of equations [4]:

$$\begin{aligned} \frac{\partial b_{k,m}(t)}{\partial t} &= \frac{-i}{2} (\delta_{m,+1} + \delta_{m,-1}) \frac{6ke^{i\omega_k t}}{(k^2 + 1)^{5/2}} F_x(t) \\ &+ \frac{(-i)^{|m-1|-|m|}}{2} F_x(t) \left(\frac{\partial}{\partial k} - ikt - \frac{m-1}{k} \right) b_{k,m-1}(t) \\ &+ \frac{(-i)^{|m+1|-|m|}}{2} F_x(t) \left(\frac{\partial}{\partial k} - ikt + \frac{m+1}{k} \right) b_{k,m+1}(t), \quad (4) \end{aligned}$$

where $\omega_k = (k^2 + 1)/2$ is the frequency of transition from the ground state to the continuous spectrum state. The initial condition for unknown amplitudes is $b_{k,m}(0) = 0$.

To solve system (4), the non-stationary perturbation theory is used, i.e. $b_{k,m}(t)$ is written as a perturbation theory series:

$$b_{k,m}(t) = \sum_{s=1,2,\dots} b_{k,m,10}^{(s)}(t),$$

where the subscript „10“ indicates the initial bound state of the electron and $b_{k,m,10}^{(s)} \sim F_0^s$.

Note that in (3) the bond with the atomic core is completely ignored.

3. Wave function in the vicinity of the center of vortex

Consider the case of steady-state solution $t > T$ and choose the following parameters of the laser pulse: $w = \pi$, $\alpha = 0$ and $T = 3, 4$. We have previously identified well localized quantum vortices specifically with these parameters [4]. In case of the even duration T , one pair of vortices appears in the momentum space, and two pairs appear for the odd duration.

Case $T = 4$. In this case, for the complete identification of quantum vortices, it is sufficient to solve system (4) to the second-order in perturbation theory. By performing this simple procedure for the chosen laser parameters, we obtain the following wave function of the photoelectron:

$$\begin{aligned} \tilde{\Psi}_4(k, \varphi_k, t) &= A \frac{\sin(k^2 + 1)}{(k^2 + 1)^{3/2}} e^{ik^2 - iE_k t} \left[\frac{k \cos(\varphi_k)}{(k^2 + 1)^2 - 4\pi^2} \right. \\ &\times \left(1 + \frac{2iF_0 k \cos(\varphi_k) (7(k^2 + 1)^2 - 4\pi^2)}{(k^2 + 1)^2 ((k^2 + 1)^2 - 16\pi^2)} \right) \\ &\left. - \frac{2iF_0}{(k^2 + 1)((k^2 + 1)^2 - 16\pi^2)} \right], \quad (5) \end{aligned}$$

where A is the constant. Here, terms with F_0 correspond to the second order in perturbation theory and the terms that are free from this amplitude correspond to the first order. Subscript „4“ indicates the excitation laser pulse duration.

The centers of quantum vortices symmetric about the k_x axis may be found from the zero equality of the real and imaginary parts of the wave function (5), i.e.

$\text{Re}(\tilde{\Psi}_4(\mathbf{k}, t)) = 0 = \text{Im}(\tilde{\Psi}_4(\mathbf{k}, t))$ (compare with [8–10]). Hence, the Cartesian and polar coordinates of the centers of vortices are equal to (Figure 1, a)

$$\begin{aligned} k_{x_0} &= 0, \quad k_{y_0} = \pm \sqrt{2\pi - 1} \approx 2.3, \\ k_0 &= \sqrt{2\pi - 1}, \quad \varphi_0 = \pi/2, 3\pi/2. \quad (6) \end{aligned}$$

„Symmetric“ flow

$$\vec{\mathbf{j}}(\mathbf{k}, t) = \text{Im}[\tilde{\Psi}^*(\mathbf{k}, t) \nabla_k \tilde{\Psi}(\mathbf{k}, t)], \quad (7)$$

where $\nabla_k \equiv \partial/\partial \mathbf{k}$ plotted for state (5) demonstrates twisting around the axis through these centers [3,4] (Figure 1, c, d).

It is easy to verify that in this case the mean momentum of the photoelectron in state (5) is equal to zero:

$$\langle k_{x,y} \rangle_4 = \int k_{x,y} |\tilde{\Psi}_4(\mathbf{k}, t)|^2 \frac{d^2 k}{2\pi} = 0, \quad (8)$$

where $k_x = k \cos(\varphi_k)$, $k_y = k \sin(\varphi_k)$.

If we go back to the taken pulse parameters, then this result seems natural. However, it should be considered that the used wave function (3) has been obtained by dropping the bound state of electron and replacing the Coulomb waves with cylindrical ones.

Mathematically, expression (8) contains the following integrals:

$$\int_0^{2\pi} \cos(\varphi_k) \cos(n\varphi_k) d\varphi_k, \quad \int_0^{2\pi} \sin(\varphi_k) \cos(n\varphi_k) d\varphi_k,$$

that in our case $n = 0, 2, 4$ make it vanish.

Dispersion of any of the momentum components is nonzero:

$$\langle k_{x,y}^2 \rangle_4 = \int k_{x,y}^2 |\tilde{\Psi}_4(\mathbf{k}, t)|^2 \frac{d^2 k}{2\pi} \neq 0. \quad (9)$$

It is impossible to calculate integral (9) analytically. Compare below the numerical values of integral (9) with the approximately found values.

Despite a relatively simple form of the wave function (5), when attempting to write it in the coordinate representation, you face significant difficulties in the Hankel transform [11]. This is the reason why the investigation of vortices in a conventional space has been performed only by means of numerical solution of the Schrödinger equation.

We will be interested hereinafter in the photoelectron behavior in the vicinity of the centers of quantum vortices. For this, expand wave function (5) in a Taylor series in the vicinity of k_0 . Thus, for individual functions from (5) we have

$$\begin{aligned} \sin(k^2 + 1) &\approx (k^2 - k_0^2), \\ \frac{1}{(k^2 + 1)^{3/2} (k^2 + (2\pi + 1))} &= e^{-\ln[(k^2 + 1)^{3/2} (k^2 + (2\pi + 1))]} \\ &\approx \frac{1}{8\sqrt{2}\pi^{5/2}} e^{-\frac{k^2 - k_0^2}{\pi}}, \end{aligned}$$

$$\frac{1}{(k^2 + 1)^{5/2}((k^2 + 1)^2 - 16\pi^2)} = e^{-\ln[(k^2+1)^{5/2}((k^2+1)^2-16\pi^2)]} \approx -\frac{1}{48\sqrt{2}\pi^{9/2}} e^{-\frac{k^2-k_0^2}{\pi}}. \quad (10)$$

Note that $((k^2+1)^2 - 4\pi^2) = (k^2 - k_0^2)(k^2 + (2\pi + 1))$ and omit the small term proportional to $\cos^2(\varphi_k)$ ($\varphi_k \approx \varphi_0$).

Then photoelectron wave function (5) in the vicinity of the center of vortex will be written as:

$$\tilde{\Psi}_{4,ap}(k, \varphi_k, \tau) = A e^{-\frac{a(\tau)}{2\sqrt{\pi}}k^2} \left[k \cos(\varphi_k) + \frac{iF_0(k^2 - k_0^2)}{3\pi^2} \right], \quad (11)$$

where $a(\tau) = (2 + i\pi\tau)/\sqrt{\pi}$, $\tau = (t - 4/2)$.

Obtained expression (11) is a Gaussian function multiplied by the second-order polynomial with respect to the momentum components (the added subscript „ ap “ is the abbreviation of „approximation“). From the structure of this polynomial, it is easy to define wave function zeroes corresponding to the centers of vortices (k_0, φ_0) (6).

Calculating the mean photoelectron momentum using (11), we can see that, as in the „precise“ wave function case (5), it is equal to zero $\langle k_{x,y} \rangle_{4,ap} = 0$. For dispersion, we obtain the following expressions:

$$\langle k_x^2 \rangle_{4,ap} = \frac{\pi}{4} \frac{[27\pi^5 + F_0^2(4 - 8\pi + 6\pi^2)]}{9\pi^5 + 2F_0^2(2 - 6\pi + 5\pi^2)} \approx \frac{3\pi}{4},$$

$$\langle k_y^2 \rangle_{4,ap} = \frac{\pi}{4} \frac{[9\pi^5 + F_0^2(4 - 8\pi + 6\pi^2)]}{9\pi^5 + 2F_0^2(2 - 6\pi + 5\pi^2)} \approx \frac{\pi}{4}. \quad (12)$$

It can be seen that the dependence on the field strength is very weak. Comparing the approximated dispersion values (12) with the corresponding numerical values obtained using (5), the latter are approximately 1.2 times as high as the former.

The key advantage of expression (11) compared with its precise equivalent (5) is in that it is easily rewritable in the coordinate representation. Without getting into specifics of simple calculations, write the answer:

$$\psi_4(r, \varphi, \tau) = \int_0^\infty \int_0^{2\pi} \tilde{\Psi}_{4,ap}(k, \varphi_k, \tau) e^{ikr \cos(\varphi_k - \varphi)} \times \frac{kdkd\varphi_k}{(2\pi)^2} = \frac{\tilde{A}}{|a(\tau)|^3} e^{-\frac{r^2}{|a(\tau)|^2} + i\frac{\pi r^2 \tau}{2|a(\tau)|^2}} \times [(F_0(4(\pi - 1) + \pi^2(r^2 - k_0^2\tau^2)) - 6\pi^3 r \cos(\varphi)) + i\pi\tau(2F_0(3\pi - 2) - 3\pi^3 r \cos(\varphi))], \quad (13)$$

where \tilde{A} is the constant, $\mathbf{r} = (r, \varphi)$ are the polar coordinates of the photoelectron and $|a(\tau)|^2 = (4 + \pi^2\tau^2)/\pi$.

Using (13), we easily find the mean photoelectron coordinates and coordinate dispersion:

$$\langle x \rangle_4 \approx -\frac{12k_0^2}{9\pi^5} F_0, \quad \langle y \rangle_4 = 0.$$

$$\langle (\Delta x)^2 \rangle_4 = \langle x^2 \rangle_4 - \langle x \rangle_4^2 \approx \frac{3\pi\tau^2}{4},$$

$$\langle (\Delta y)^2 \rangle_4 = \langle y^2 \rangle_4 - \langle y \rangle_4^2 \approx \frac{\pi\tau^2}{4}. \quad (14)$$

Whereby, as must be the case, $|a(\tau)|^2 \approx \langle (\Delta x)^2 \rangle_4 + \langle (\Delta y)^2 \rangle_4$.

The obtained wave function in the coordinate representation (13) has a similar structure with the wave function in the momentum representation (11). The Gaussian multiplier describes the spreading of the formed wave packet. The second-order polynomial with respect to the photoelectron coordinates contains the information about the quantum vortex in the conventional space. By setting the real and imaginary parts of the expression in brackets in (13) to zero and solving the derived system of equations, we find the coordinates of the centers of vortices:

$$x_0 = \frac{F_0(6\pi - 4)}{3\pi^3},$$

$$y_0 = \pm \sqrt{\frac{k_0^2 |a(\tau)|^2}{\pi} - x_0^2} \approx \pm k_0\tau. \quad (15)$$

From (15) we draw obvious conclusions: vortex moves at a velocity equal to k_0 that defines zero of the wave function in the momentum space; for the given even T , the vortex will move along the axis perpendicular to the linear polarization of the ionizing field. This indicates indirectly that the nature of vortices is attributed to the interference of states assigned to opposite waves.

Case $T = 3$. In case of odd duration $T = 3$, the photoelectron wave function obtained considering the second-order in perturbation theory is written as

$$\tilde{\Psi}'_3(k, \varphi_k, t) = A \frac{e^{-iE_k t}}{(k^2 + 1)^{7/2}} \times \left[\frac{8i\pi^4 e^{\frac{3}{4}i(k^2+1)}(k^2 + 1)^2 \cos(\frac{3}{4}(k^2 + 1))k \cos(\varphi_k)}{(k^2 + 1)^2 - 4\pi^2} - \frac{4\pi^2 F_0}{(k^2 + 1)^4 - 20\pi^2(k^2 + 1)^2 + 64\pi^4} \left[k^2 \cos(2\varphi_k) \times (((k^2 + 1)^2 - 9\pi^2)(k^2 + 1)^2 + \pi^2 e^{\frac{3}{2}i(k^2+1)}) \times (4\pi^2 - 7(k^2 + 1)^2) - 4\pi^4 \right] + (4\pi^4 k^2 - \pi^2 e^{\frac{3}{2}i(k^2+1)}) \times ((5k^2 - 2)(k^2 + 1)^2 + 4\pi^2(k^2 + 2)) + (k^2 + 1)^2 \times (k^6 + 2k^4 - 11\pi^2 k^2 + k^2 - 2\pi^2) + 8\pi^4 \right]. \quad (16)$$

As in the previous case, wave function (16) makes it possible to identify zeroes corresponding to the centers of vortices [4]. There are four such zeroes whose Cartesian coordinates are

$$k_{x_{01}} = 0, \quad k_{y_{01}} = \pm \sqrt{4\pi/3 - 1} \approx \pm 1.79,$$

$$k_{x_{02}} = 0, \quad k_{y_{02}} = \pm \sqrt{8\pi/3 - 1} \approx \pm 2.72. \quad (17)$$

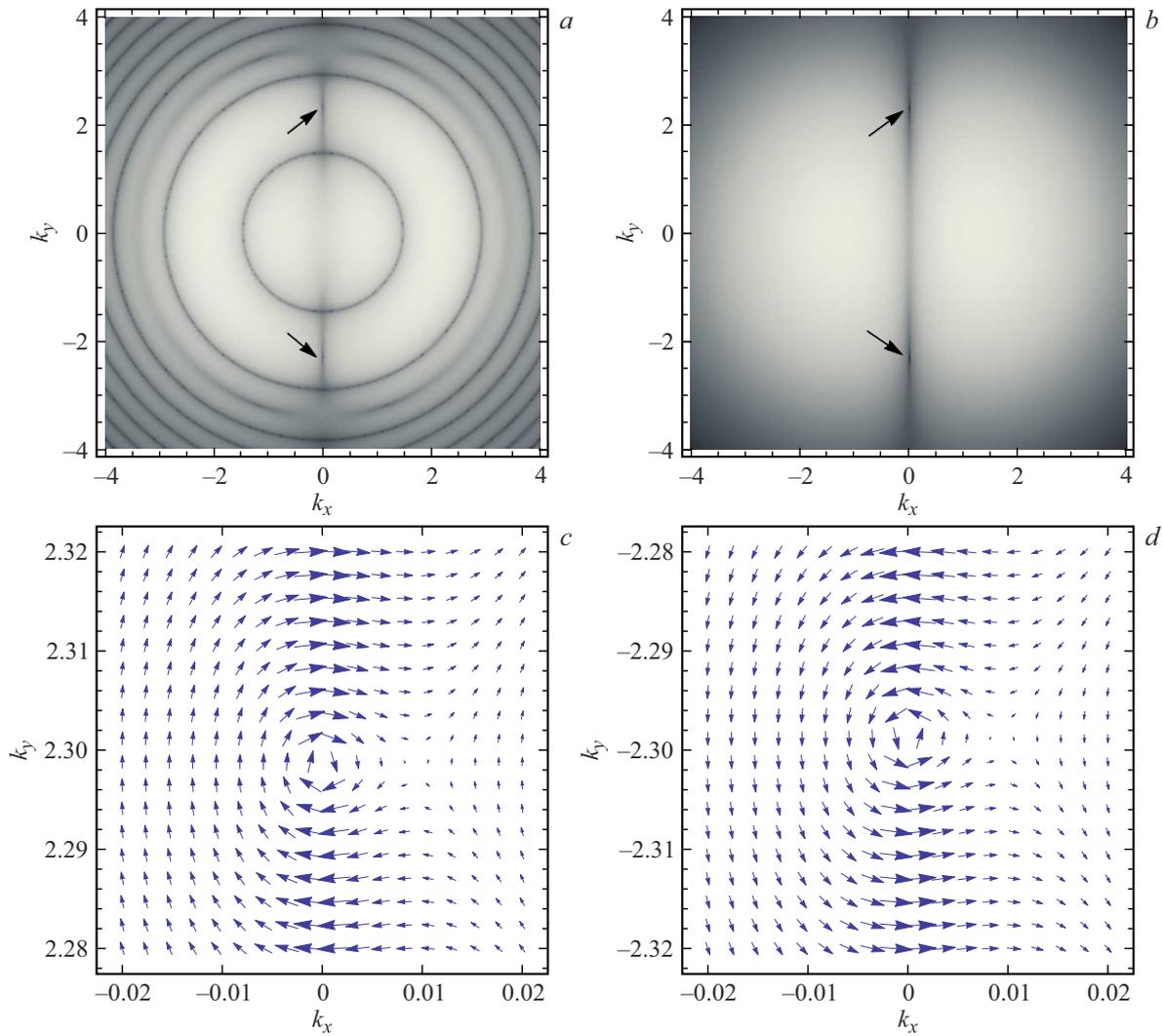


Figure 1. Photoelectron momentum density $\ln[\rho(k_x, k_y)]$: $a - \rho(\mathbf{k}) = |\tilde{\Psi}_4(\mathbf{k}, t)|^2$, $b - \rho(\mathbf{k}) = |\tilde{\Psi}_{4,ap}(\mathbf{k}, t)|^2$. c and d — vector field $\bar{\mathbf{v}}(k_x, k_y, t)$ in the vicinity of the centers of quantum vortices. Pulse duration $T = 4$. Laser field strength $F_0 = 0.4$ and $t = 5$.

Polar coordinates are

$$\begin{aligned} k_{01} &= \sqrt{4\pi/3 - 1}, \quad \varphi_{01} = \pi/2, 3\pi/2, \\ k_{02} &= \sqrt{8\pi/3 - 1}, \quad \varphi_{02} = \pi/2, 3\pi/2. \end{aligned} \quad (18)$$

That is there are two pair of quantum vortices symmetric about the k_x axis.

However, the „symmetric“ flow (7) plotted using (16) will not demonstrate any vortex behavior around the centers of these vortices. Here, for the given case of the odd T , the third order in perturbation theory must be considered. To avoid overloading the text, the third-order correction $\delta\tilde{\Psi}_3(k, \varphi_k, t)$ to (16) is removed into the Appendix.

$$\tilde{\Psi}_3(k, \varphi_k, t) = \tilde{\Psi}'_3(k, \varphi_k, t) + \delta\tilde{\Psi}_3(k, \varphi_k, t) \quad (19)$$

Now we will be interested in the behavior of wave function (19) in the vicinity of two neighboring vortices (Figure 2).

If we do the same as in the case with $T = 4$, i.e. expand the wave function in a Taylor series in the vicinity of one of the centers, then we lose the information about the neighboring second vortex. Therefore, we will perform the expansion in the vicinity of the resonance value $k_r = \sqrt{2\pi - 1}$ that lies exactly almost between the centers of two neighboring vortices $\sqrt{4\pi/3 - 1} < k_r < \sqrt{8\pi/3 - 1}$ (for $T = 4$ the value of k_r coincided with the coordinate of the center of vortex k_0).

Performing expansion $\tilde{\Psi}_3(k, \varphi_k, t)$ (19) sequentially, as in the previous case, in the vicinity of k_r , we derive the following simplified expression:

$$\begin{aligned} \tilde{\Psi}_{3,ap}(k, \varphi_k, \tau') &= A e^{-\frac{a(\tau')}{2\sqrt{\pi}} k^2} \left[\left(1 - \frac{F_0^2}{2\pi^3} \right. \right. \\ &\left. \left. - i \left(\frac{4}{9\pi^4} + \frac{3}{8\pi^2} \right) F_0^2 \right) k \cos(\varphi_k) - \frac{4F_0(1 - \frac{9}{32}(k^2 - k_r^2)^2)}{9\pi^2} \right], \end{aligned} \quad (20)$$

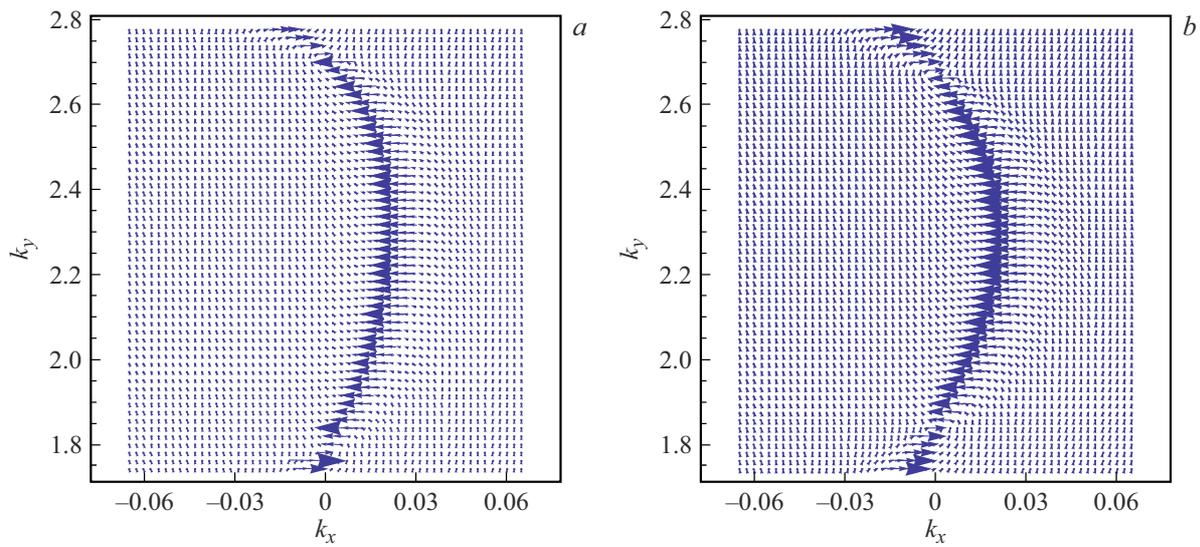


Figure 2. *a* and *b* — vector field $\vec{v}(k_x, k_y, t)$ in the vicinity of the centers of quantum vortices. Pulse duration — $T = 3$. Laser field strength — $F_0 = 0.5$ and $t = 4$.

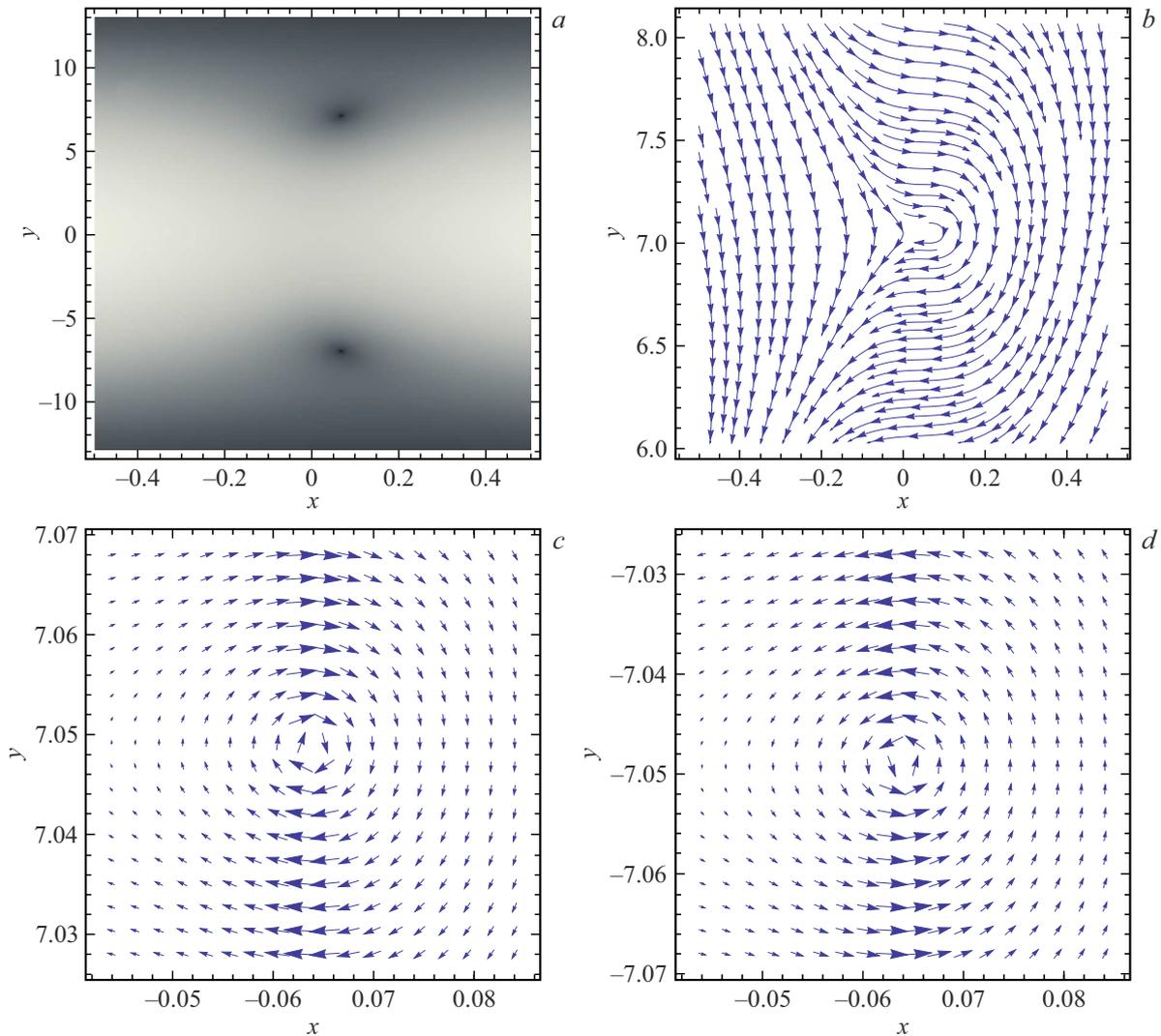


Figure 3. *a* — Photoelectron density $\ln[\rho(x, y, t)]$. *b, c, d* — vector field $\mathbf{v}(x, y, t)$ in the vicinity of the centers of quantum vortices. Pulse duration $T = 4$. Laser field strength — $F_0 = 0.4$. Time $t = 5$.

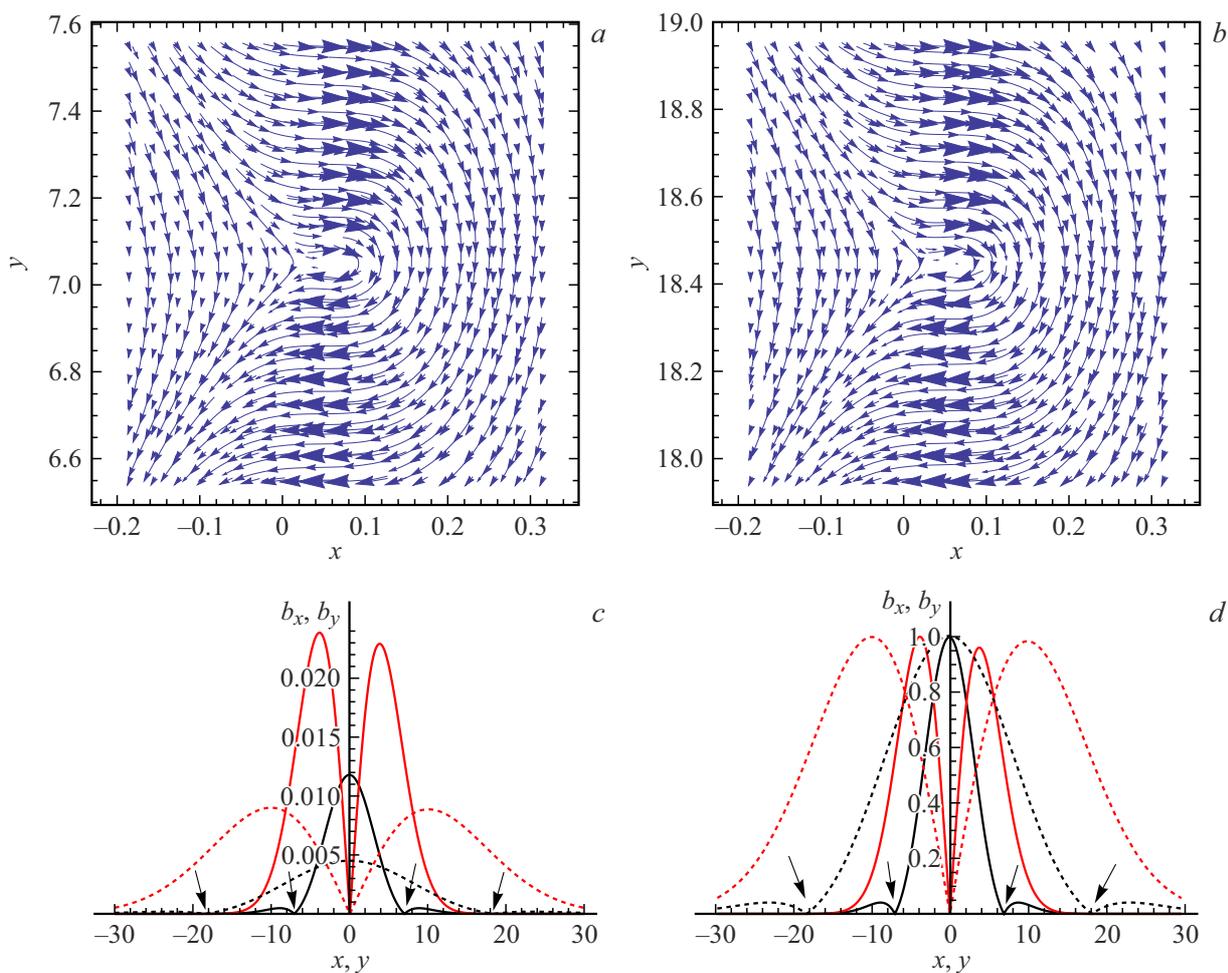


Figure 4. Vector field $v(x, y, t_i)$ in the vicinity of the centers of quantum vortices in different times: $a - t_1 = 5$, $b - t_2 = 10$. c, d — absolute values of the wave function b_x (red curve), b_y (black curve) vs. the x, y components, respectively: $t_1 = 5$ — solid line, $t_2 = 10$ — dashed line. Arrows indicate the centers of vortices. Pulse duration $T = 4$. Laser field strength $F_0 = 0.4$.

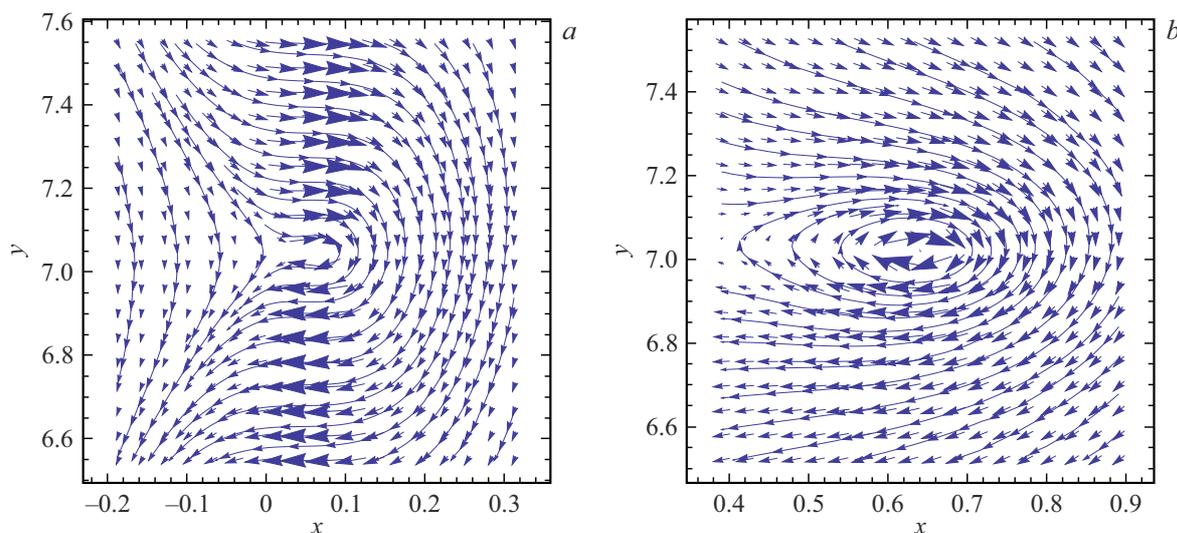


Figure 5. Vector field $v(x, y, t_i)$ in the vicinity of the center of the quantum vortex: $a - F_0 = 0.4$, $x_0 = 0.064$, $y_0 = 7.049$; $b - F_0 = 4$, $x_0 = 0.639$, $y_0 = 7.02$. Pulse duration $T = 4$. Time $t = 5$.

where the terms with F_0^2 correspond to the third order in perturbation theory and $a(\tau') = (2 + i\pi\tau')/\sqrt{\pi}$, $\tau' = t - 3/2$.

In the same way as for $T = 4$, the polynomial at the Gaussian function allows the coordinates of the centers of vortices to be found easily. However, here, due to the chosen expansion point, they are shifted a little along the k_y axis

$$\begin{aligned} k'_{01} &= \sqrt{k_r^2 - 4\sqrt{2}/3} \approx 1.84 \approx k_{01}, \\ k'_{02} &= \sqrt{k_r^2 + 4\sqrt{2}/3} \approx 2.68 \approx k_{02}. \end{aligned} \quad (21)$$

Calculating the momenta observed in state (20) (or (19)), it can be seen that the mean momentum of the photoelectron along the x axis is nonzero, i.e. $\langle k_x \rangle_{3,ap} \neq 0$, $\langle k_y \rangle_{3,ap} = 0$. This, as in the case described above, may be explained by the given pulse parameters.

We will not write the explicit expressions for mean $\langle k_x \rangle_{3,ap}$ and $\langle k_{x,y}^2 \rangle_{3,ap}$ calculated using (20) due to their awkwardness. We should note only that these expressions give results that qualitatively coincide with the results calculated using the „precise“ wave function $\tilde{\Psi}_3(k, \varphi_k, t)$ (19).

By applying the Fourier transform to (20), we obtain the corresponding function in the coordinate representation:

$$\begin{aligned} \psi_3(r, \varphi, \tau') &= \int_0^\infty \int_0^{2\pi} \tilde{\Psi}_{3,ap}(k, \varphi_k, \tau') e^{ikr \cos(\varphi_k - \varphi)} \\ &\times \frac{k dk d\varphi_k}{(2\pi)^2} = \frac{\tilde{A}}{|a(\tau')|^5} e^{-\frac{r^2}{|a(\tau')|^2} + i\frac{\pi r^2 \tau'}{2|a(\tau')|^2}} \\ &\times \left[ia^3(\tau') \left(1 - \frac{F_0^2}{2\pi^3} - i \left(\frac{4}{9\pi^4} + \frac{3}{8\pi^2} \right) F_0^2 \right) r \cos(\varphi) \right. \\ &\left. + \frac{F_0}{8\pi^{1/2}} \left(r^4 + c_1(\tau')r^2 + c_2(\tau') \right) \right], \end{aligned} \quad (22)$$

where coefficients $c_i(\tau')$ are removed to the Appendix due to their awkwardness.

Function (22) has an expected structure similar to the one that took place for $T = 4$. However, the polynomial at the Gaussian exponent that defines the centers of vortices in the conventional space, has a more complicated structure than in (13). Therefore, we will not write the zeroes of this polynomial.

Quantum vortices in the coordinate space will be investigated in the next section using obtained wave functions (13) and (22).

4. Calculation results

Momentum space. First we will check how the probability density has changed during the wave function expansion in

the vicinity of the center of the vortex. Recall that the time t is taken everywhere such that $t > T$.

Figure 1 for $T = 4$ shows the photoelectron momentum distribution $\rho(\mathbf{k})$ (for more explicit display, the diagrams are plotted for $\ln(\rho)$) plotted using the „precise“ wave function $\tilde{\Psi}_4(\mathbf{k}, t)$ (5) (Figure 1, *a*) and its approximation $\tilde{\Psi}_{4,ap}(\mathbf{k}, t)$ (11) (Figure 1, *b*).

Expansion (10) applied to $\tilde{\Psi}_4(\mathbf{k}, t)$ (5) has led to the loss of information about the photoelectron states away from the centers of quantum vortices. However, this information is still preserved in the immediate vicinity to them, which is evident not only from the probability density zeroes (arrows), but also from the nature of the vector field for the normalized „symmetric“ flow (7) (Figure 1, *c, d*)

$$\bar{\mathbf{v}}(\mathbf{k}, t) = \bar{\mathbf{j}}(\mathbf{k}, t)/\rho(\mathbf{k}). \quad (23)$$

The field $\bar{\mathbf{v}}(\mathbf{k}, t)$ obtained using only approximate function (11) is represented here. For the chosen range of values of k_x, k_y , it will be no different from the field plotted using the „precise“ function (5) [4].

Note that the top and bottom vortices are absolutely the same, except that their directions of rotation are opposite. Also note that, due to free movement of the photoelectron, the momentum density $\rho(\mathbf{k})$ is written without the argument t . When it comes to the „symmetric“ flow (7), due to its sensitivity to the wave function phase [5], the time dependence is retained.

The vector field $\bar{\mathbf{v}}(\mathbf{k}, t)$ for $T = 3$ is shown in Figure 2. The upper half-plane, where one pair of vortices is localized, is addressed.

When using the „precise“ wave function $\tilde{\Psi}_3(\mathbf{k}, t)$ (19), the coordinates of the centers of vortices are given by equation (17) or (18) (Figure 2, *a*). For approximate function $\tilde{\Psi}_{3,ap}(\mathbf{k}, t)$ (20), these coordinates are shifted a little (21) (Figure 2, *b*).

Momentum densities $\rho(\mathbf{k})$ plotted using functions (19) and (20) will differ from each other in the same manner as in the case with $T = 4$ (Figure 1, *a, b*).

Coordinate space. Figure 3 for $T = 4$ shows the photoelectron distribution $\rho(\mathbf{r}, t) = |\psi_4(\mathbf{r}, t)|^2$ (Figure 3, *a*) and photoelectron velocity field (Figure 3, *b, c, d*)

$$\mathbf{v}(\mathbf{r}, t) = \text{Im}[\psi_4^*(\mathbf{r}, t)\nabla\psi_4(\mathbf{r}, t)]/\rho(\mathbf{r}, t) \quad (24)$$

(the term „velocity field“ was borrowed from the quantum hydrodynamics [12–14]) plotted using derived wave function (13).

As for the momentum space, there are two symmetric vortices with opposite directions of rotation (Figure 3, *c, d*). Coordinates of the centers of vortices are given by equations (15) and equal to $x_0 = 0.064$, $y_0 = \pm 7.049$.

Note that the found vortices in the momentum and coordinate spaces correspond to each other. However, the real structure of vortices in the coordinate space corresponding to the „precise“ function (5) will differ from that in the momentum space. Dropping in (5) of the term

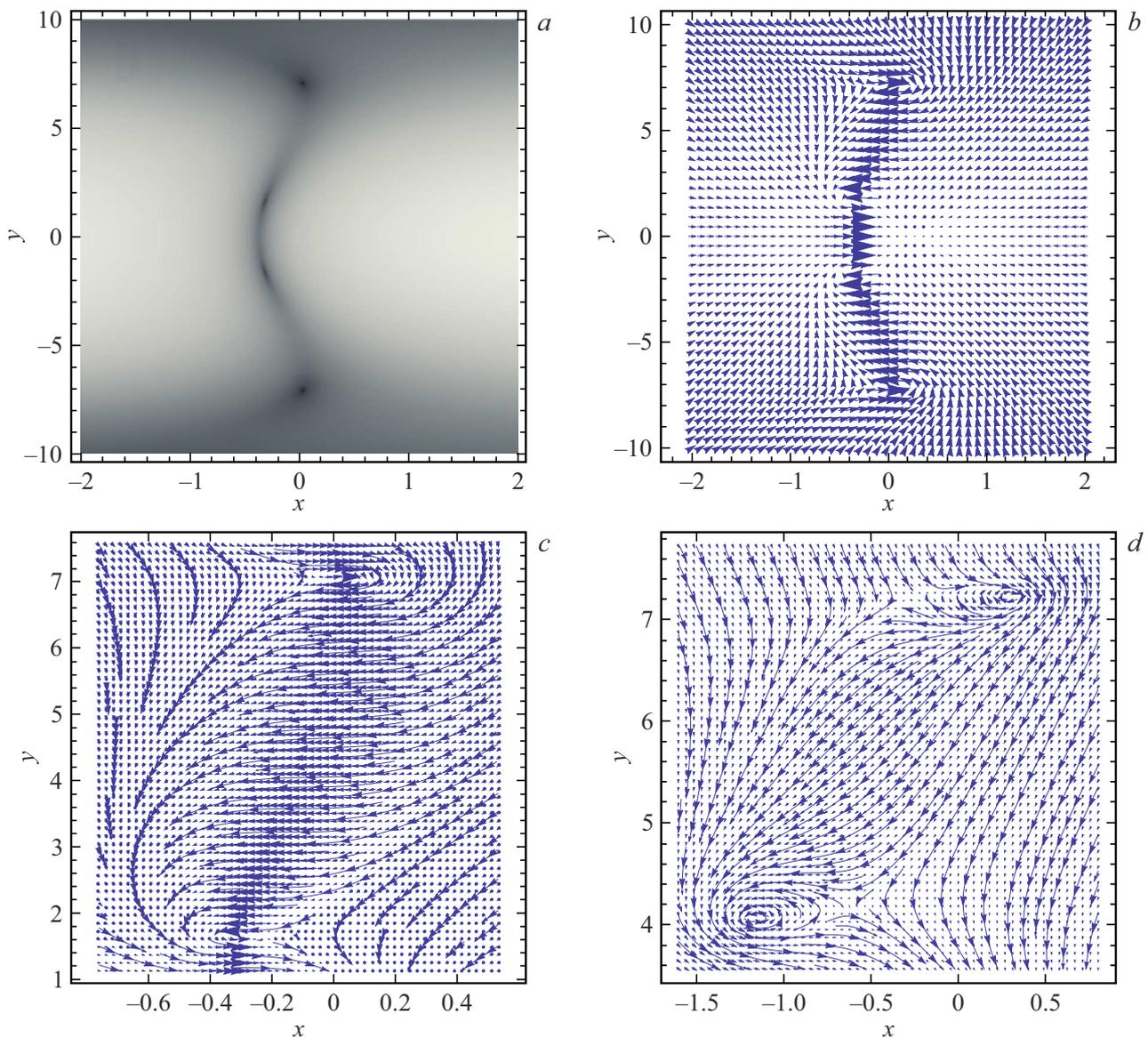


Figure 6. *a* — Photoelectron density $\ln[\rho(x, y, t)]$, *b* — corresponding vector field $\mathbf{v}(x, y, t)$. *c, d* — vector field $\mathbf{v}(x, y, t)$ in the vicinity of the centers of neighboring vortices. *a, b, c* — $F_0 = 0.5$. *d* — $F_0 = 5$. Pulse duration $T = 3$. Time $t = 4$.

with $\cos^2(\varphi_k)$ and approximation of rational functions of k by the Gaussian function erase the information about the photoelectron behavior outside the vortex localization area. At the same time, the Fourier transform covers all possible values of \mathbf{k} .

Now we shall trace the time evolution of the vortices. Figure 4 for two different times $t_1 = 5$, $t_2 = 10$ shows the field $\mathbf{v}(x, y, t_i)$ and the following dependences of the wave function modulus $b_x(t_i) \equiv |\psi(x, y_0, t_i)|$, $b_y(t_i) \equiv |\psi(x_0, y, t_i)|$ on one of the coordinates (Figure 4, *d* — normalized to their peaks of function $b_{x,y}$).

It can be seen that wave packet spreading shown by the curves in Figure 4. *c, d* does not change the geometry and scale of the vortex in Figure 4. *a, b*. The vortex moves in space without changes and the coordinate of its center is

described by equation (15): $t_1 - x_0 = 0.064$, $y_0 = \pm 7.049$; $t_2 - x_0 = 0.064$, $y_0 = \pm 18.446$.

In the following Figure 5, the photoelectron velocity field $\mathbf{v}(x, y, t)$ is plotted at different strengths F_0 of the ionizing laser pulse. Here, taking into account the suddenness of field inclusion (2), we go beyond small perturbations [15].

We can see that the increase in the field strength F_0 leads to the increase in the vortex scale. The plotted current lines clearly demonstrate that in case of high strength F_0 the velocity field $\mathbf{v}(x, y, t)$ will have a solenoid structure at much larger scales than in case of low strengths.

Figure 6 shows the results obtained using the wave function $\psi_3(x, y, \tau')$ (22). Zeroes in the photoelectron distribution (Figure 6, *a*) that correspond to the centers of

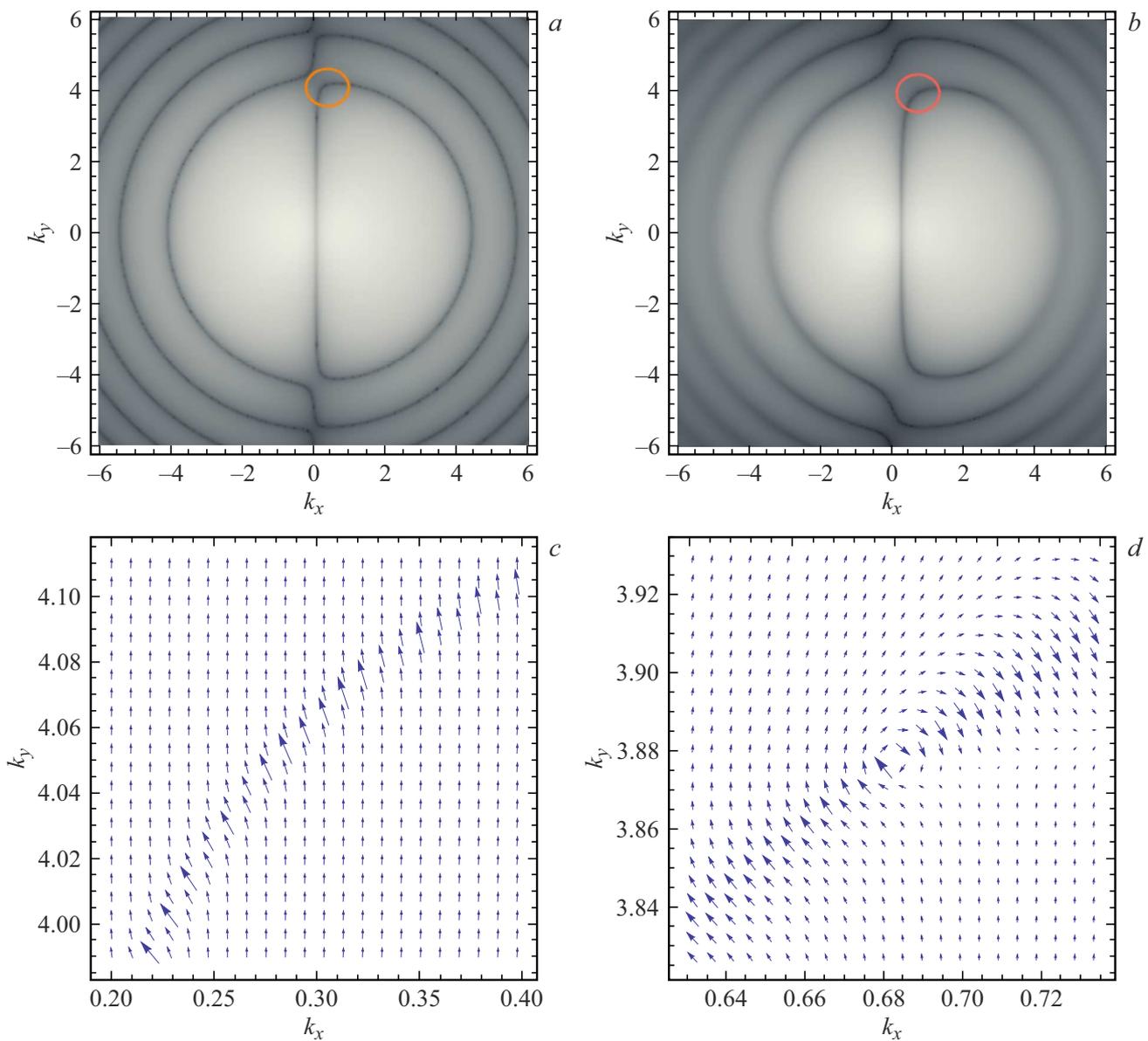


Figure 7. *a, b* — Photoelectron momentum density $\ln[\rho(k_x, k_y)]$. *c, d* — vector field $\mathbf{v}(k_x, k_y, t)$ in the circled area in *a, b*. *a, c* — $F_0 = 0.5$. *b, d* — $F_0 = 2$. Pulse duration $T = 1$. Time $t = 2$.

two pairs of vortices are clearly seen. Figure 6, *b* shows the corresponding velocity field $\mathbf{v}(x, y, t)$ twisted around each of these centers. The direction of vortex rotation is the same as in the momentum space: a pair of vortices in the upper half-plane with the opposite direction of rotation and a pair in the lower half-plane that is symmetric to it about the x axis.

The coordinates of the centers of vortices are found by setting the real and imaginary parts of the polynomial to zero in wave function expression (22). For the case shown in Figure 6 with the given $t = 4$ we have: $F_0 = 0.5$: $x_{01} = -0.31$, $y_{01} = \pm 1.63$, $x_{02} = 0.034$, $y_{02} = \pm 7.05$; $F_0 = 5$: $x_{01} = -1.16$, $y_{01} = \pm 4.07$, $x_{02} = 0.3$, $y_{02} = \pm 7.22$.

As for the even T , the increase in strength leads to the increase in the vortex scale (Figure 6, *c, d*).

The explicit time dependence of the coordinates of the centers of vortices in case of $\psi_3(x, y, \tau')$ (22) has a complex form and cannot be reduced to simple motion similar to (15).

In spreading of the wave packet corresponding to $\psi_3(x, y, \tau')$ (22), the vortices are retained.

Duration $T = 1$. As noted earlier [2,3], with the pulse duration equal to half-period, i.e. $T = 1$, for $F_0 < 1$ no vortices are observed. On the other hand, as shown above, the increase in the field amplitude F_0 leads to the increase in the vortex scale. Therefore it is interesting to consider the case with $T = 1$ for different values of F_0 .

Figure 7 at $T = 1$ and two different strengths $F_0 = 0.5, 2$ shows the photoelectron momentum distribution $\rho(\mathbf{k})$ and vector field $\bar{\mathbf{v}}(\mathbf{k}, t)$. It can be seen that the increase in the field strength leads to formation of vortices (Figure 7, *d*). This is a manifestation of the well-known dependence of transition probability on the field intensity and the time of exposure of this field to the quantum system [15].

With $F_0 = 0.5, T = 1$ is not sufficient to provide electron transition from the bound state to the continuous spectrum states responsible for vortex formation [4]. The increase in strength compensates this short duration and the probability of transition to the required states increases.

As mentioned above, to identify vortices in the case with $T = 3$ (Figure 2), the third order in perturbation theory shall be considered. However, according to the preliminary calculations, if $F_0 > 1$ is taken, then the vortices may be already seen in the second order.

5. Conclusion

In this work, a wave function describing quantum vortices was obtained for a photoelectron torn out from a two-dimensional hydrogen atom by an extremely short laser pulse. The analytical expression of this wave function both in the momentum and coordinate representation has a simple form — the Gaussian function multiplied by the polynomial with respect to the photoelectron coordinates. The polynomial contains information about the centers of quantum vortices and is responsible for vortex behavior of the photoelectron velocity field, and the Gaussian function describes spreading of the formed wave packet.

The obtained wave function made it possible to investigate the quantum vortex evolution in the coordinate space: the vortex moves in space without distortions at a velocity defined by zero of the wave function in the momentum space corresponding to the center of quantum vortex.

It is shown that the vortex scale formally defined as the region where the velocity vector field is close to the solenoid field may be changed by varying the electric field strength of the ionizing pulse. In particular, the short pulse duration with which the vortices fail to form may be compensated by the increase in the field strength.

Note that the strong field limit $F_0 > 1$ addressed here certainly required a more rigorous approach. Moreover, the approximations that were used initially have essentially reduced the considered problem of the photoelectron to the analysis of a specific state of a free particle that depends on the strength F_0 as on an external parameter.

Conflict of interest

The authors declare that they have no conflict of interest.

Appendix

Third-order correction to the photoelectron wave function (16):

$$\begin{aligned} \delta\tilde{\Psi}_3(k, \varphi_k, t) = & A \frac{e^{-iE_k t}}{(k^2 + 1)^{7/2}} \\ & \times \frac{-iF_0^2 e^{\frac{3}{4}i(k^2+1)} k \cos(\varphi_k)}{((k^2 + 1)^2 - 4\pi^2)^2 ((k^2 + 1)^4 - 52\pi^2(k^2 + 1)^2 + 576\pi^4)} \\ & \times \left[\cos\left(\frac{3}{4}(k^2 + 1)\right) (16\pi^2 - (k^2 + 1)^2) \right. \\ & \times \left[-4k^2(k^2 + 1)^6 - i\pi^2(3(k^2 + (2 + 40i))k^2 + (3 + 16i)) \right. \\ & \times (k^2 + 1)^4 + 24\pi^4(k^2 + 1)^2(5ik^4 - (6 - 10i)k^2 \\ & + (12 + 5i)) - 16i\pi^6(27k^4 + (54 - 4i)k^2 + (27 - 24i)) \\ & - 4k^2((k^2 + 1)^6 - 26\pi^2(k^2 + 1)^4 + 108\pi^4(k^2 + 1)^2 \\ & \left. \left. - 80\pi^6) \cos(2\varphi_k) \right] - \sin\left(\frac{3}{4}(k^2 + 1)\right) ((k^2 + 1)^4 \right. \\ & \left. - 40\pi^2(k^2 + 1)^2 + 144\pi^4) \left[4ik^2(k^2 + 1)^4 - \pi^2(k^2 + 1)^2 \right. \right. \\ & \times (3(k^2 + (2 + 8i))k^2 + (3 + 16i)) + 16\pi^4(3k^4 \\ & + (6 + 2i)k^2 + (3 + 4i)) + 4ik^2((k^2 + 1)^4 \\ & \left. \left. - 2\pi^2(k^2 + 1)^2 - 8\pi^4) \cos(2\varphi_k) \right] \right]. \end{aligned} \quad (25)$$

Coefficients included in the photoelectron wave function in the coordinate representation (22):

$$\begin{aligned} c_1(\tau') &= \frac{2k_r^2 a^2(\tau')}{\pi} - \frac{8a(\tau')}{\pi^{1/2}}, \\ c_2(\tau') &= \frac{(36\pi^2 - 36\pi - 23)a^4(\tau')}{9\pi^2} \\ &\quad - \frac{4k_r^2 a^3(\tau')}{\pi^{3/2}} + \frac{8a^2(\tau')}{\pi}. \end{aligned} \quad (26)$$

References

- [1] N.V. Larionov, D.N. Makarov, A.A. Smirnovsky, S.Yu. Ovchinnikov. *J. Exp. Theor. Phys.*, **129**, 949 (2019). DOI: 10.1134/S1063776119110062
- [2] S.Yu. Ovchinnikov, N.V. Larionov, A.A. Smirnovsky, A.A. Shmidt. *St. Petersburg Polytechnical State University Journal. Physics and Mathematics*, **10**, 111 (2017). DOI: 10.18721/JPM.10409
- [3] N.V. Larionov, V.M. Molchanovskiy. *Opt. Spectrosc.*, **132**, 387 (2024). DOI: 10.1134/S0030400X24040118
- [4] N.V. Larionov *ZhETF* **165**, 317 (2024) (in Russian). DOI: 10.31857/S0044451024030027
- [5] R.F. Nalewajski. *J. Math. Chem.*, **53**, 1966 (2015). DOI: 10.1007/s10910-015-0526-2

- [6] V.M. Galitsky, B.M. Karnakov, V.I. Kogan. *Zadachi po kvantovoy mekhanike: uchebnoe posobie dlya vuzov* (Nauka, Moskva, 1992).
- [7] M.V. Fedorov. J. Exp. Theor. Phys., **122**, 449 (2016). DOI: 10.1134/S1063776116030043
- [8] S.Y. Ovchinnikov, J. Sternberg, J. Macek, T.-G. Lee, D.R. Schultz. Phys. Rev. Lett., **105**, 203005 (2010). DOI: 10.1103/PhysRevLett.105.203005
- [9] F. Navarrete, R. Della Picca, J. Fiol, R.O. Barrachina. J. Phys. B: At. Mol. Opt. Phys., **46**, 115203 (2013). DOI: 10.1088/0953-4075/46/11/115203
- [10] S.Y. Ovchinnikov, J.H. Macek, D.R. Schultz. Phys. Rev. A, **90**, 062713 (2014). DOI: 10.1103/PhysRevA.90.062713
- [11] V.A. Ditkin, A.P. Prudnikov. *Integral Transformations and Operational Calculus* (Pergamon Press, 1965).
- [12] E. Madelung. Z. Phys., **40**, 332–326 (1926).
- [13] T. Takabayashi. Prog. Theor. Phys., **8**, 143 (1952).
- [14] A. Visinescu, D. Grecu, R. Fedele, S. De Nicola. Theor. Math. Phys., **160**, 1066–1074 (2009). DOI: 10.1007/s11232-009-0098-z
- [15] L.D. Landau, E.M. Lifshitz. Course of Theoretical Physics, Vol. 3: Quantum Mechanics: Non-Relativistic Theory (Fizmatlit, Moscow, 2004; Pergamon, New York, 1977, 3rd ed.).

Translated by E.Ilinskaya