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Identification of quantum vortices in momentum space

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The quantum vortices formed as a result of barrier-suppression ionization of a two-dimensional hydrogen atom by an ultrashort laser pulse are theoretically investigated. Using an analytical expression for the wave function of a photoelectron in the momentum representation, the probability flux density is investigated. In this case, both the standard definition of a flux and an alternative „symmetrical" one are used. The latter, due to the sensitivity to the phase of the wave function, makes it possible to identify quantum vortices in the momentum space.

Keywords: quantum vortex, momentum representation, probability flux.

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Introduction

One of the nontrivial effects that arise during the ionization of an atom is the formation of quantum vortices [1–10]. These vortices manifest themselves as perturbations in the probability density for the photoelectron. The center of the vortex is a region forbidden for the photoelectron and probability flux circulates around it.

In [4–6], using both numerical and analytical approaches, we studied the formation and evolution of quantum vortices formed in above-barrier ionization of a two-dimensional hydrogen atom by an ultrashort laser pulse. The analytical approach was based on solving the Schrödinger equation using nonstationary perturbation theory. The wave function of the photoelectron was obtained, which was successfully used for identification of the centers of quantum vortices and further comparison with numerical calculations. However, the vector field of the probability flux has not been analyzed with its help. Here we fill this gap, using both the standard expression for flux in momentum space and an alternative expression that is sensitive to the phase of the wave function. This alternative „flux" was introduced in work [11] and is a quantity „symmetric" with respect to the flux written in position space.

Theoretical model

We will use a system of atomic units in which the Schrödinger equation for a two-dimensional hydrogen atom interacting with a laser pulse has the form

$$i\,\frac{\partial}{\partial t}|\Psi(t)\rangle=(\hat{H}_0+\hat{V})|\Psi(t)\rangle, \tag{1}$$

where $\hat{H}_0$ — Hamiltonian of a free atom, $\hat{V}=-\hat{\mathbf{d}}\mathbf{F}(t)$ — operator of interaction of an atom with the electric field of a laser $\mathbf{F}(t)$, $\hat{\mathbf{d}}=-\hat{\mathbf{r}}$ — dipole moment operator.

As in previous works [4–6], we will look for a solution to equation (1) in the strong field approximation. This means that in the calculations we will neglect the excited states of the atom and will not take into account the Coulomb effect on the photoelectron. We will also assume that changes in the population of the ground (initial) state of the atom are negligible. Then the solution to the Schródinger equation (1) can be written as the following superposition:

$$|\Psi(t)|=|\Psi^{(0)}_{1,0}\rangle e^{-iE_1t}+\sum_{m=0,\pm1,\ldots}\int\limits_0^\infty b_{k,m}(t)|\Psi^{(0)}_{k,m}\rangle e^{-iE_kt}kdk. \tag{2}$$

Here the first term corresponds to the ground state of the atom with energy $E_1=-1/2$, characterized by the vector $|\Psi^{(0)}_{1,0}\rangle$. Subscripts „$1,0$" indicate the values of the principal quantum number $n=1$ and the projection of the moment onto the axis z $m=0$. The second term is represented by a superposition of photoelectron state vectors $|\Psi^{(0)}_{k,m}\rangle$, which we will describe by cylindrical waves. The indices „k,m" indicate that this state is characterized by the energy $E_k=k^2/2=(k_x^2+k_y^2)/2$ and the projection of the moment $m=0,\pm1,\pm2,\ldots$.

Since our task is to identify quantum vortices in momentum space, we rewrite (2) in the appropriate representation:

$$\Psi(\mathbf{k},t)\equiv\langle\mathbf{k}|\Psi(t)\rangle=\frac{2}{(k^2+1)^{3/2}}\Phi_0(\varphi_k)e^{-iE_1t}+\sum_{m=0,\pm1,\ldots}b_{k,m}(t)(-i)^{|m|}\Phi_m(\varphi_k)e^{-iE_kt}, \tag{3}$$

where $\mathbf{k}=(k,\varphi_k)$ — electron momentum in the polar coordinate system, $\Phi_m(\varphi_k)=e^{im\varphi_k}/\sqrt{2\pi}$, and explicit expressions were used for the wave functions in the momentum representation [6]:

$$\Psi^{(0)}_{1,0}(\mathbf{k})\equiv\langle\mathbf{k}|\Psi^{(0)}_{1,0}\rangle=\frac{2\Phi_0(\varphi_k)}{(k^2+1)^{3/2}},$$

$$\Psi^{(0)}_{k',m}(\mathbf{k}) \equiv \langle \mathbf{k}|\Psi^{(0)}_{k',m}\rangle = (-i)^{|m|}\frac{\delta(k'-k)}{k'}\,\Phi_m(\varphi_k). \quad (4)$$

Expansion (3) allows us to derive a closed equation for the unknown coefficients $b_{k,m}(t)$. For this, let us substitute (3) (or (2)) into the Schrödinger equation (1). Then, taking into account the explicit form of the interaction operator in the momentum representation:

$$\hat{V} = \mathbf{F}(t)i\partial/\partial\mathbf{k},$$

we obtain

$$\frac{\partial b_{k,m}(t)}{\partial t} = \frac{(-i)}{2}(\delta_{m,1}+\delta_{m,-1})F_x(t)\,\frac{6ke^{i\omega_{k1}t}}{(k^2+1)^{5/2}}$$
$$+\frac{(-i)^{|m-1|-|m|}}{2}F_x(t)\left(\frac{\partial}{\partial k} - ikt - \frac{m-1}{k}\right)b_{k,m-1}(t)$$
$$+\frac{(-i)^{|m+1|-|m|}}{2}F_x(t)\left(\frac{\partial}{\partial k} - ikt + \frac{m+1}{k}\right)b_{k,m+1}(t), \quad (5)$$

where $\omega_{k1} = (k^2+1)/2$ and the field polarized along the x axis is considered $\mathbf{F}(t) = (F_x(t), 0)$. The system of equations (5) corresponds to the system we obtained earlier in the work [6]. The difference is more convenient recording without introducing characters $\pm$, $\mp$.

Solving system (5) using perturbation theory, the following expression can be obtained for the part of the wave function (3) corresponding to the continuous spectrum:

$$\tilde{\Psi}(\mathbf{k},t) = -i\left[b^{(1)}_{k-1,10}(t)\Phi_{-1}(\varphi_k) + b^{(1)}_{k1,10}(t)\Phi_1(\varphi_k)\right]e^{-iE_kt}$$
$$+ b^{(2)}_{k0,10}(t)\Phi_0(\varphi_k)e^{-iE_kt}$$
$$-\left[b^{(2)}_{k-2,10}(t)\Phi_{-2}(\varphi_k) + b^{(2)}_{k2,10}(t)\Phi_2(\varphi_k)\right]e^{-iE_kt}, \quad (6)$$

where the superscript of the amplitudes corresponds to the order of perturbation theory [5,6], and the added subscript „10" indicates the initial bound state of the electron. The tilde sign over Ψ emphasizes (in [5,6] the notation $\tilde{\Psi}(\mathbf{k}.t) = b(\mathbf{k},t)e^{-iE_kt}$ was adopted) that the bound state is omitted, i.e. in the further consideration, the interference between the initial and final states of the electron is neglected.

Our task is to identify quantum vortices in momentum space. For it, we will use the following two definitions for the probability flux in momentum space $\mathbf{k}$:

$$\mathbf{j}(\mathbf{k},t) = \mathbf{k}|\tilde{\Psi}(\mathbf{k},t)|^2,$$
$$\bar{\mathbf{j}}(\mathbf{k},t) = -\frac{1}{2i}\left[\tilde{\Psi}^*(\mathbf{k},t)\nabla_k\tilde{\Psi}(\mathbf{k},t) - \tilde{\Psi}(\mathbf{k},t)\nabla_k\tilde{\Psi}^*(\mathbf{k},t)\right]. \quad (7)$$

Here $\mathbf{j}(\mathbf{k},t)$ — standard expression for the probability flux in momentum space, $\bar{\mathbf{j}}(\mathbf{k},t)$ — „symmetric" probability flux [11], where $\nabla_k = \partial/\partial\mathbf{k}$.

As shown earlier [5,6], quantum vortices that appear during the ionization of an atom are caused by the interference of photoelectron states. Therefore, in order to correctly describe these vortices, it is required to know the phase of the wave function. Let us highlight this phase in the found wave function (6):

$$\tilde{\Psi}(\mathbf{k},t) = |\tilde{\Psi}(\mathbf{k},t)|e^{i\chi(\mathbf{k},t)},$$

where $\chi(\mathbf{k},t)$ — phase. If we substitute $\tilde{\Psi}(\mathbf{k},t)$ into the standard definition of the probability flux $\mathbf{j}(\mathbf{k},t)$, then the $\chi(\mathbf{k},t)$ phase will disappear, and identification of the quantum vortex will be possible mainly by the zeros of the wave function. The situation is different for the alternative stream $\bar{\mathbf{j}}(\mathbf{k},t)$. In fact, substituting $\tilde{\Psi}(\mathbf{k},t)$ into the expression for $\bar{\mathbf{j}}(\mathbf{k},t)$, we obtain

$$\bar{\mathbf{j}}(\mathbf{k},t) = -|\tilde{\Psi}(\mathbf{k},t)|^2\nabla_k\chi(\mathbf{k},t).$$

Calculation results and discussion

We simulate the non-zero component of the laser pulse field strength with the following expression:

$$F_x(t) = F_0\cos(\omega t)[\theta(T-t) - \theta(-t)], \quad (8)$$

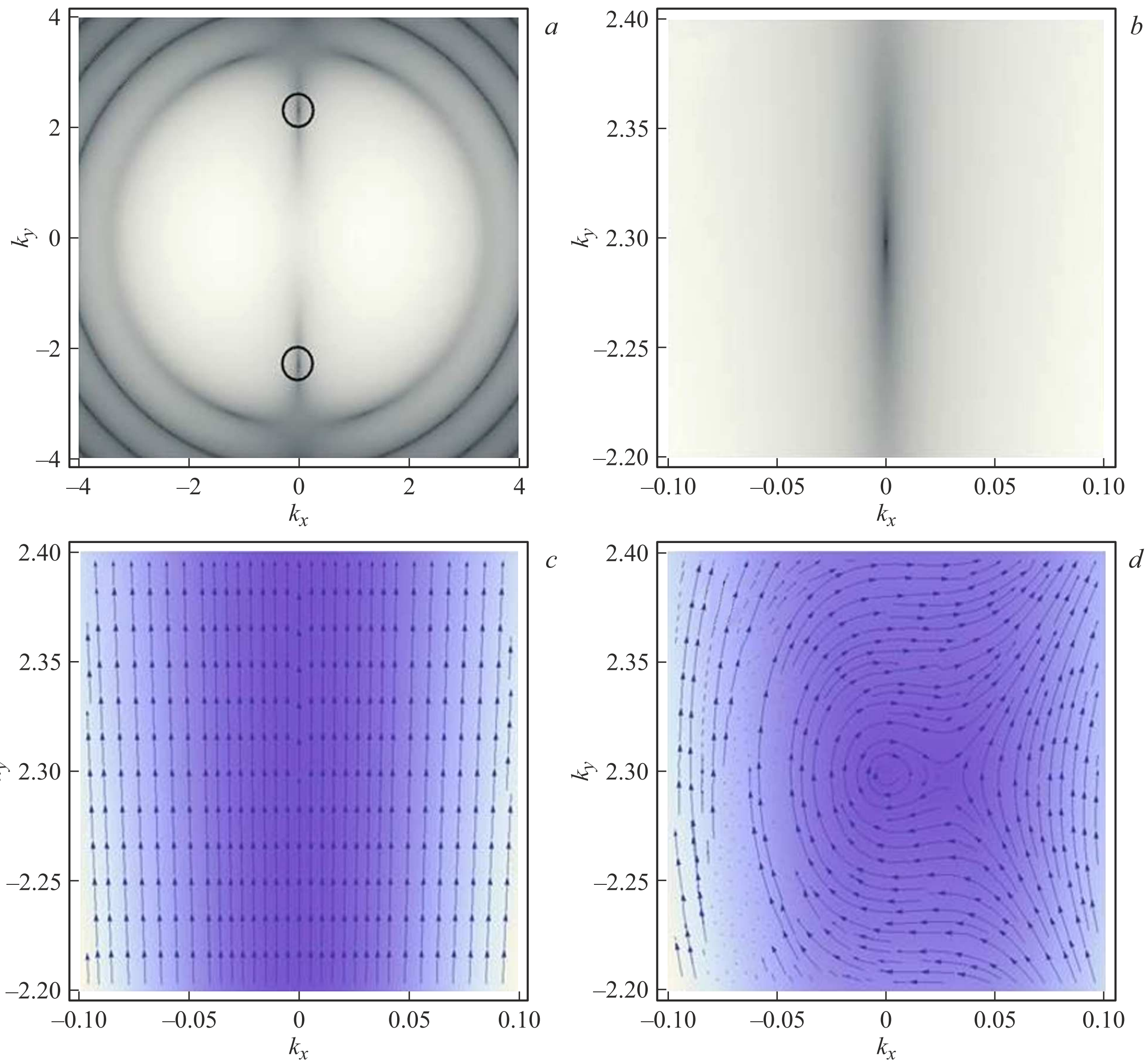
where $\theta(x)$ — Heaviside function, F_0 — constant amplitude, ω — frequency, T — pulse duration. We choose the values of the pulse parameters close to those for which quantum vortices were previously identified [4–6]: $F_0 = 0.6$, $\omega = \pi$, $T = 2$. We will be interested in the steady-state solution, i.e. explore $\tilde{\Psi}(\mathbf{k},t)$ (6) at times $t > T$.

Let us make a few comments regarding the selected parameters. The field amplitude value is taken such that above-barrier ionization predominates, but meanwhile $F_0 < 1$. This allows to remain within the limits of the theoretical approximations used. The „scale" of the vortex is strongly influenced by the pulse duration T [4]. As calculations show, at $T < 1$ the vortex does not have time to form and it cannot be identified. When going to large values of $T > 10$, the forbidden region gradually „smears out", and ultimately the vortex loses its individuality, and the „picture " becomes similar to that which occurs during ionization by a monochromatic field.

The figure shows graphs of the photoelectron momentum distribution $|\tilde{\Psi}(k_x,k_y,t>T)|^2$ (a,b) (for a clearer display, the graph is plotted for $\ln|\tilde{\Psi}|^2$) and the standard probability flux $\mathbf{j}(k_x,k_y,t>T)$ (c) and „symmetric" flux $\bar{\mathbf{j}}(k_x,k_y,t>T)$ (d).

For the selected parameters there are two symmetrical vortices with centers at points $k_x = 0$, $k_y \approx \pm 2.3$. In the figure, *a* these centers are highlighted with circles, and in the figure, *b* the center of the vortex with the positive coordinate $k_y \approx 2.3$ is shown on an enlarged scale.

Figure, *c* illustrates the standard probability flux in momentum space. It can be seen that in the vicinity of the center of the vortex $k_x = 0$, $k_y \approx 2.3$ the flux is not distinguished in any way and coincides with the average flux in this region of momentum space. Only the darker



Distribution of photoelectron momenta (a, b), standard probability flux (c) and „symmetric“ flux (d).

background on the graph indicates the presence of a forbidden region for the photoelectron.

The „symmetric“ flux looks completely different, figure *d*. It is clearly seen that around the zero of the wave function the flux $\bar{\mathbf{j}}(k_x, k_y, t > T)$ has a vortex structure close to solenoidal.

Conclusion

Thus, it is shown that using the symmetric expression for the probability flux $\bar{\mathbf{j}}(\mathbf{k}, t)$ (7), introduced in [11], quantum vortices in momentum space are possible to be identified.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] F. Cajiao Véez, LeiGeng, J.Z. Kamińki, Liang-You Peng, K. Krajewska. Phys. Rev. A, **102**, 043102 (2020). DOI: 10.1103/PhysRevA.102.043102

[2] F. Cajiao Vélez. Phys. Rev. A, **104**, 043116 (2021). DOI: 10.1103/PhysRevA.104.043116

[3] Lei Geng, F. Cajiao Vélez, J.Z. Kamiński, Liang-You Peng, K. Krajewska. Phys. Rev. A, **104**, 033111 (2021). DOI: 10.1103/PhysRevA.104.033111

[4] S.Yu. Ovchinnikov, N.V. Larionov, A.A. Smirnovsky, A.A. Schmidt. St.Petersburg Polytechnical St. University J. Phys. Math., **10** (4), 111–121 (2017). DOI: 10.18721/JPM.10409

[5] N.V. Larionov, A.A. Smirnovsky, S.Y. Ovchinnikov, A.A. Schmidt. Tech. Phys., **63** (11), 1569–1575 (2018). DOI: 10.1134/S1063784218110166

[6] N.V. Larionov, A.A. Smirnovsky, D.N. Makarov, S.Y. Ovchinnikov. JETP, **129** (6), 949–955 (2019). DOI: 10.1134/S1063776119110062
[7] J.H. Macek, J.B. Sternberg, S.Y. Ovchinnikov, J.S. Briggs. Phys. Rev. Lett., **104** (3), 033201 (2010). DOI: 10.1103/PhysRevLett.104.033201
[8] F. Navarrete, R. Della Picca, J. Fiol, R.O. Barrachina. J. Phys. B, **46** (11), 115203 (2013). DOI: 10.1088/0953-4075/46/11/115203
[9] F. Navarrete, R.O. Barrachina. Nucl. Instr. Meth. Phys. Res. B, **369**, 72–76 (2016). DOI: 10.1016/j.nimb.2015.09.073.
[10] C.M. DeMars, S.J. Ward, J. Colgan, S. Amami, D.H. Madison. Atoms, **8** (2), 26 (2020). DOI: 10.3390/atoms8020026
[11] R.F. Nalewajski. J. Math. Chem., **53**, 1966–1985 (2015). DOI: 10.1007/s10910-015-0526-2

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