Validity of the Wannier threshold law for angular correlation width in double photoionization of atoms

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We calculated using the *ab initio* method the three-fold differential cross section of a single-photon double photoionization of helium at equal energy sharing and derived the Gaussian width parameter γ , describing the angular interelectron correlations, for the total electron energy *E* ranging from 0.1 to 100 eV. The results are in perfect agreement with experimental data. Contrary to common expectations, the results demonstrate that the Wannier threshold law for the Gaussian width parameter $\gamma \propto E^{1/4}$ is not correct at energies attainable in modern experiments. It is shown that the γ dependence on the energy is much better described by the modified threshold law, obtained by Kazansky and Ostrovsky [J. Phys. B **26**[, 2231 \(1993\)\]](http://dx.doi.org/10.1088/0953-4075/26/15/010). Also, we explored the Gaussian width parameter for double photoionization of targets with strongly asymmetrical initial-state configuration: the atomic hydrogen negative ion H[−] and the helium atom in the $2s¹S$ and $3s¹S$ excited states. We found that the Gaussian width dependence on the total ejected electron energy for these targets has a maximum at low energies. We also show that the correlation parameter dependence on the interelectron angle for these targets is essentially non-Gaussian and has a number of peaks equal to the number of the initialstate radial nodes, which provide new facilities for the qualitative analysis of the electron structure of the target atom.

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I. INTRODUCTION

Interelectron correlations are principal components in many processes in atomic physics, chemistry, and plasma and solid state physics. The problem of two free electrons moving in the Coulomb field of a third body can be treated as a fundamental problem for investigation of interelectron correlations because they are not negligible in such a process. More than 50 years ago, Wannier [\[1\]](#page-6-0) showed that, if two slow electrons escape from the residual positively charged core, then, independent of how the electrons are released, the cross section of the two-electron ejection would be *^σ* [∝] *^E^α*, where *α >* 1 depends only on the residual ion charge and E is the total energy of the electrons. He obtained this expression having divided the space surrounding the ion into three regions: the reaction zone (where the electrons start), the Coulomb zone (where the potential energy of the interaction between the electrons and the ion is much larger than *E*), and the free zone (where *E* is much larger than the Coulomb potential). The behavior of the electrons in the Coulomb zone was considered as classical. It also follows from his theory that the electrons should predominantly go in opposite directions. For a long time, only total cross sections have been explored both in experiment and theory until the appearance of the experimental facilities based on the coincidence technique, allowing the measurement of momenta of all outgoing particles. This enables one to study the multifold differential cross sections that depend on the electron energy sharing and electron ejection angles and yield significant information about the interelectron correlations.

One of the simplest processes caused by the interelectron correlations is the helium double ionization by a single photon [\[2\]](#page-6-0). It is known that, if the incident radiation is linearly polarized in the *Oz* direction, the three-fold differential cross section (3DCS) of the double photoionization of an atom by a single photon can be represented via gerade and ungerade amplitudes [\[3\]](#page-6-0)

$$
\frac{d^3\sigma}{dE_1 d\Omega_1 d\Omega_2} = |a_g(E_1, E_2, \theta_{12})(\cos\theta_1 + \cos\theta_2) + a_u(E_1, E_2, \theta_{12})(\cos\theta_1 - \cos\theta_2)|^2, \quad (1)
$$

where E_1 and E_2 are energies of the ejected electrons, θ_{12} is an angle between directions of ejection, and the ungerade amplitude $a_u = 0$ for $E_1 = E_2$. The gerade amplitude a_g is usually referred to as the correlation parameter. Following Wannier's theory [\[1\]](#page-6-0), the interelectron potential can be approximated by the quadratic term in its Taylor series with respect to $(\theta_{12} - \pi)$ in the vicinity of the saddle point $(\theta_{12} = \pi, r_1 = r_2)$, i.e., by the harmonic-oscillator potential with the frequency, depending on the hyperradius $R = \sqrt{r_1^2 + r_2^2}$. Rau [\[4\]](#page-6-0) assumed that the wave-function angular behavior near the saddle point coincides with the oscillator ground mode for each *R* value inside the Coulomb zone, and in the free zone it "freezes" and coincides with the oscillator ground mode at the boundary between the Coulomb and the free zones. This leads to the Gaussian shape for the correlation parameter [\[5\]](#page-6-0):

$$
a_g(E_1, E_2, \theta_{12}) \simeq A \exp \left[-2 \ln 2 \frac{(\theta_{12} - \pi)^2}{\gamma^2} \right],
$$
 (2)

with the Gaussian width parameter equal to

$$
\gamma = \gamma_0 E^{1/4},\tag{3}
$$

where $E = E_1 + E_2$ is the energy excess above the doubleionization threshold, and the scaled Gaussian width γ_0 depends on the choice of the hyperradius of the boundary between the Coulomb and free zones. By analogy with the Wannier threshold law for the cross section, Eq. (3) is also commonly referred to as the Wannier threshold law, although Wannier himself has no direct relation to it. The Gaussian width parameter γ is a single-angle parameter describing the angular distribution. When γ is large, the interelectron correlation is weak, and vice versa; therefore, it is often used for the analysis of the strength of angular interelectron correlation. In spite of the fact that the energy range, where Eq. [\(3\)](#page-0-0) is valid, is not established, experimenters and theorists often use Eq. [\(3\)](#page-0-0) for the data interpretation, trying to find the scaled width parameter γ_0 . Many formulas for γ_0 have been proposed by various authors [\[6\]](#page-6-0). However, Kazansky and Ostrovsky [\[7\]](#page-6-0) reduced the problem by a change of variable to the wave-packet evolution in a harmonic oscillator with time-dependent frequency and showed that the packet width has no time to follow adiabatically the oscillator frequency as a result of the deceleration of electrons by the nucleus field. This contradicts the assumption used in $[5]$ to obtain (3) , and when the nonadiabaticity is taken into account, the near-threshold behavior of Gaussian width is strongly modified. They also showed that the assumption about the presence of the only oscillator ground mode at the boundary of the reaction zone is not true and, therefore, $a_g(\theta_{12})$ depends on the details of the process inside the reaction zone and can have non-Gaussian shape even at $E \to 0$.

The initial reason that motivated us to start this work was that we have found $\lceil 8 \rceil$ that γ for the hydrogen negative ion H[−] starts to grow with energy decreasing at low energies, in obvious contradiction with the Wannier threshold law. In trying to explain this phenomenon, we explored the wellknown and seemingly understood problem of the Gaussian width parameter energy dependence for a helium atom at low energies. The work structure is as follows. In Sec. II, we describe the calculation method, the problems appearing during the calculations, the parameters used in the calculations, and the methods of the extraction of the Gaussian width parameter γ from the calculated 3DCS. In Sec. III, the results of the calculations of the Gaussian width parameter *γ* for single-photon double photoionization of a helium atom are given. The obtained results are compared with the Wannier threshold law and the near-threshold results of Kazansky and Ostrovsky. In Sec. [IV,](#page-2-0) we compare the differential cross sections and *γ* for single-photon double photoionization of H[−] and He in $2s¹S$ and $3s¹S$ excited states, and discuss the origin of difference in shapes of γ dependences on energy for these targets from those for He and positive He-like ions.

II. DETAILS OF THE CALCULATION PROCEDURE

In our calculations, we used the time-dependent scaling (TDS) method [\[8,9\]](#page-6-0). The main advantage of this method is the possibility of obtaining the 3DCS for all values of the ingoing photon energy in a single run of the program. As a result, we obtain a continuous dependence of 3DCS upon the energy, whereas other widespread *ab initio* methods imply a separate calculation for each value of energy. Unfortunately, along with the component corresponding to the double ionization and described correctly in the expanding coordinate system, the wave function also comprises the components that describe the bound states and the single-ionization states, which are poorly described at large values of the expansion coefficient $a(t)$ (see [\[9\]](#page-6-0)). At evolution times $t \gg 1000$, this gives rise

to noise-looking short-period oscillations, the wavelength of which becomes comparable to the radial grid step *h*. Note that oscillations in $\gamma(E)$ have been observed in some other calculations [\[10\]](#page-6-0). However, there is enough evidence to support that the oscillations mentioned in this paper are numerical artifacts caused by the bound-state destruction: (1) when the grid step is changed, the oscillation wavelength follows it; (2) the oscillations always appear when $a(t)h$ approaches the typical bound-state radius and spreads toward the increasing radius. For this reason, we filtered the wave function after the evolution by eliminating all components with wavelengths less than 4*h*. We should note that, even without filtration, there are no oscillations in our calculations in the energy range where the oscillations in convergent close-coupling (CCC) calculations [\[10\]](#page-6-0) appear.

In the calculations of helium photoionization presented in this paper, we used the following numerical scheme parameters (see [\[8\]](#page-6-0) for details): the angular basis parameter $l_{2\text{max}} = 13$, the uniform radial grid with $N_r = 500$ and the size $\xi_{\text{max}} = 25$, the complex scaling radius $\xi_{\text{sc}} = 22.5$, the complex scaling angle $\theta_{\rm sc} = 30^\circ$, and the grid expansion rate $a_{\infty} = 0.1$. The evolution was simulated up to the time $t_{\text{max}} = 12800$. For other targets, other radial grid parameters are used: $N_r = 500$, $\xi_{\text{max}} = 50$, $\xi_{\text{sc}} = 45$, $\dot{a}_{\infty} = 0.05$ for H−, *Nr* = 1000, *ξ*max = 50, *ξ*sc = 40, and *a*˙[∞] = 0*.*05 for the He in the excited $1s2s¹S$ state; and $N_r = 1400$, $\xi_{\text{max}} = 70$, $\xi_{\rm sc} = 60$, and $\dot{a}_{\infty} = 1/30$ for He in the 1*s*3*s*¹*S* state.

The calculated 3DCS is then used to derive the Gaussian width parameter γ . The squared module of the correlation parameter $|a_g(E_1, E_1, \theta_{12})|^2$ may be extracted from the 3DCS using Eq. (1) and then approximated by Eq. (2) using the least-squares (LS) method [\[11\]](#page-6-0). An alternative approach [\[12\]](#page-6-0) is based on approximating the calculated two-fold differential cross section (2DCS) $\sigma^{(2)}(E_1, E_2, \theta_{12}) = \frac{d^2\sigma}{dE_1 d\theta_{12}}$ by the expansion

$$
\sigma^{(2)}(E_1, E_1, \theta_{12}) \simeq \frac{32\pi^2}{3} |A|^2 \exp\left[-\frac{4\ln 2(\pi - \theta_{12})^2}{\gamma^2}\right] \cos^2 \frac{\theta_{12}}{2},\tag{4}
$$

which is derived from Eq. [\(1\)](#page-0-0) by integrating over all angles except θ_{12} . The values of 3DCS near $\theta_{12} = \pi$ contribute to the sum of squares in the LS method with smaller weight when fitting $\sigma^{(2)}(\theta_{12})$ than when fitting $|a_g(\theta_{12})|^2$. Since the correlation parameter $a_{\varrho}(\theta_{12})$ can noticeably deviate from the Gaussian shape, the γ values calculated using the two methods are different. The Gaussian width parameter, obtained by fitting $|a_g(\theta_{12})|^2$, will be referred to as $\gamma(|a_g|^2)$, while *γ*, obtained by fitting $\sigma^{(2)}(\theta_{12})$, will be referred to as $\gamma(\sigma^{(2)})$.

III. THE PHOTOIONIZATION OF THE HELIUM IN THE GROUND STATE

In Fig. [1,](#page-2-0) we plot the Gaussian width parameter γ as a function of the full energy of ejected electrons *E* for the double photoionization at equal energy sharing of helium in the ground state. Our results show perfect agreement with the experiment in the entire range from 0.1 to 100 eV, except for the point at 4 eV from [\[17\]](#page-6-0). The exact coincidence of our curve $\gamma(\sigma^{(2)})$ with the experimental points at 0.116 and 0.209 eV from [\[12\]](#page-6-0) is

FIG. 1. (Color online) The Gaussian width parameter *γ* as a function of the full energy of ejected electrons *E* for the photoionization of He: our results were obtained by the fitting of $\sigma^{(2)}(\theta_1)$ (thick solid line) and $|a_g(\theta_{12})|^2$ (thin solid line), along with CCC results [\[10,11\]](#page-6-0) (dashed line), TDCC results [\[13\]](#page-6-0) (dotted line), H*R*M-SOW results [\[14\]](#page-6-0) (dash-dotted line), and experimental data [\[12,15–19\]](#page-6-0) (filled circles).

the most remarkable. The curve $\gamma(|a_g|^2)$ shows less agreement with these points, which is not surprising since just $\gamma(\sigma^{(2)})$ has been obtained in the experiment [\[12\]](#page-6-0). At high energies, the experimental point at 80 eV was obtained in [\[19\]](#page-6-0) by the fitting of $|a_g(\theta_{12})|^2$ and, hence, it is not surprising that this point is much closer to our $\gamma(|a_g|^2)$ curve than to the $\gamma(\sigma^{(2)})$ curve. Generally, the differences between $\gamma(|a_g|^2)$ and $\gamma(\sigma^{(2)})$ may be a manifestation of the degree of the $a_g(\theta_{12})$ deviation from the Gaussian shape, although the coincidence of $\gamma(|a_g|^2)$ with $\gamma(\sigma^{(2)})$ does not mean that $a_{\varrho}(\theta_{12})$ is exactly Gaussian. In Fig. 1, the results of other authors' *ab initio* calculations are also shown. The agreement of the CCC results [\[10,11\]](#page-6-0) with our results is good for *E >* 10 eV and satisfactory for lower energies. The time-dependent close-coupling (TDCC) results [\[13\]](#page-6-0), where available, are close to our results, and the hyperspherical *R*-matrix with semiclassical outgoing wave (H*R*M-SOW) results [\[14\]](#page-6-0) strongly differ from all other curves.

Figure 1 is presented in logarithmic scales at both axes, in which the power dependences such as the Wannier law [\(3\)](#page-0-0) should look like sloping straight lines. Indeed, we see that our plots are close to straight lines when *E* is less than a few electron volts. However, the exponent is not equal to 1*/*4 at all. The approximation of the $\gamma(\sigma^{(2)})$ curve in the *E* range from 0.1 to 2 eV, using the power law of the general form

$$
\gamma = \tilde{\gamma}_0 E^s \tag{5}
$$

through the least-squares approach, yields the exponent $s =$ 0.097 and the proportionality constant $\tilde{\gamma}_0 = 70^\circ \text{ eV}^{-s}$. Such a significant deviation from the Wannier threshold law, which is often used for the interpretation of experimental and theoretical data, seems to be discouraging. In Fig. 2, we show the scaled width parameter $\gamma_0(E) = \gamma(E)/E^{1/4}$ in comparison with the curve obtained in [\[7\]](#page-6-0) using the quadratic approximation of the interelectron potential in $(\theta_{12} - \pi)$ and the semiclassical approximation for radial motion. We also take into account the nonadiabaticity of the wave-function angular dependence on the hyperradius and the suggestion that only the lowest mode in θ_{12} is populated at the boundary of the reaction zone with

FIG. 2. (Color online) The scaled width parameter γ_0 as a function of *E* for He: our results were obtained with the fitting of $\sigma^{(2)}(\theta_{12})$ (thick solid line) and $|a_g(\theta_{12})|^2$ (thin solid line), along with the Kasansky-Ostrovsky threshold law [\[7\]](#page-6-0) (dashed line).

the hyperradius assumed to be $R = 4$, which we will refer to as the Kasansky-Ostrovsky (KO) threshold law. It is clear that our curves are close to the KO threshold law curve, down to the minimal energy value $E = 0.1$ eV attained here. In Fig. 2, the Wannier threshold law [\(3\)](#page-0-0) would look like a horizontal straight line. At very low energies of the order of 10−⁵ eV, the KO curve seems to become horizontal, but this is just because the energies below 10−⁶ eV are not shown in the figure, as follows from [\[7\]](#page-6-0). Following the KO threshold law, $\gamma_0(E)$ oscillates when energy decreases with the period, which is constant in the logarithmic scale [\[7\]](#page-6-0) (in Fig. 2, only a half of the period is shown) and never turns into the Wannier threshold law.

IV. PHOTOIONIZATION OF THE TARGETS WITH STRONGLY ASYMMETRICAL INITIAL-STATE CONFIGURATION

In our previous work $[8]$, we compared the dependences $\gamma(E)$ for various heliumlike ions and found that, for the negative hydrogen ion H−, this function starts to increase at energies below 2.5 eV, unlike for other considered targets. We extended the results of [\[8\]](#page-6-0) down to the energy value of 0.06 eV.

FIG. 3. (Color online) The Gaussian width *γ* as a function of *E* for the photoionization of H−: our results were obtained by the fitting of $\sigma^{(2)}(\theta_{12})$ (thick solid line) and $|a_g(\theta_{12})|^2$ (thin solid line), along with the Kasansky-Ostrovsky threshold law [\[7\]](#page-6-0) (dashed line).

FIG. 4. (Color online) The 2DCS as a function of the interelectron angle θ_{12} for the photoionization of H⁻ for (a) $E = 0.1$ eV and (b) $E = 2.5$ eV: "exact" TDS results (solid line), Gaussian fitting of $\sigma^{(2)}(\theta_{12})$ (dashed line), and the Gaussian fitting of $|a_g(\theta_{12})|^2$ (dotted line).

It is clear from Fig. [3](#page-2-0) that derivative of $\gamma(\sigma^{(2)})$ with respect to the energy is negative in the energy range from 2.6 to 0.23 eV. In Fig. 4, the 2DCS dependence on the interelectron angle θ_{12} and its Gaussian fittings are shown for the *E* value below the maximum of $\gamma(E)$ [Fig. 4(a)] and near the minimum of $\gamma(E)$ [Fig. 4(b)]. At energies below 0.09 eV, $\gamma(\sigma^{(2)})$ appears to be a power function of the energy with the exponent $s = 0.083$ and $\tilde{\gamma}_0 = 74^\circ \text{ eV}^{-s}$; however, the energy range is too small to treat this conclusion as a rigorous one. Figure 5 demonstrates a clear-cut distinction between our results and the KO threshold law for the nuclear charge $Z = 1$ [\[7\]](#page-6-0), unlike the helium case (Fig. [2\)](#page-2-0). We should note that the $\gamma(E)$ dependence obtained by Kasansky and Ostrovsky is monotonous (Fig. [3\)](#page-2-0), despite the $\gamma_0(E)$ dependence oscillating. Here we should note that the KO curve is obtained from the assumption that, at the boundary of the reaction zone, only the ground angular mode is populated; but, in the same work [\[7\]](#page-6-0), it is shown that it is not necessary at all, even at $E \to 0$, and at the boundary of the reaction zone, the wave-function angular dependence may have an arbitrary width or even be non-Gaussian, depending on the details of the process inside the reaction zone. Our hypothesis is that this special feature of H−, compared with

FIG. 5. (Color online) The scaled width parameter γ_0 as a function of *E* for H[−]: our results were obtained by the fitting of $\sigma^{(2)}(\theta_{12})$ (thick solid line) and $|a_g(\theta_{12})|^2$ (thin solid line), along with the Kasansky– Ostrovsky threshold law [\[7\]](#page-6-0) (dashed line).

helium and heliumlike ions [\[8\]](#page-6-0), comes from the fact that the H[−] bound-state configuration is strongly different from that of the helium ground state. Indeed, when $r_{1,2} \rightarrow \infty$, the H⁻ bound-state wave function has the asymptotic form

$$
\Phi(\mathbf{r}_1,\mathbf{r}_2)\sim e^{-r_1}\frac{e^{-0.235r_2}}{r_2}+e^{-r_2}\frac{e^{-0.235r_1}}{r_1}.
$$

H[−] is a deuteronlike weakly bound system consisting of a hydrogen atom and an electron, spending the most time outside the region where the attracting potential acts. We performed here the calculations for other targets with strongly asymmetrical initial-state configuration, namely, helium atoms in the excited states $2s¹S$ and $3s¹S$.

In Fig. 6, we show γ as a function of *E* for the photoionization of helium in the $2s¹S$ metastable state. Our results do not deviate much from the CCC results [\[10\]](#page-6-0) in magnitude, but deviate strongly in behavior, since there are no oscillations in our results. When the energy decreases, *γ* also decreases at first and then begins to increase [for $\gamma(\sigma^{(2)})$

FIG. 6. (Color online) The Gaussian width *γ* as a function of *E* for the photoionization of $\text{He}(2s¹S)$: our results were obtained by the fitting of $\sigma^{(2)}(\theta_{12})$ (thick solid line) and $|a_g(\theta_{12})|^2$ (thin solid line), along with CCC results [\[10\]](#page-6-0).

FIG. 7. (Color online) The 2DCS as a function of the interelectron angle θ_{12} for the photoionization of He(2*s*¹*S*) for (a) $E = 1$ eV, (b) $E = 11$ eV, and (c) $E = 20$ eV: "exact" TDS results (solid line), Gaussian fitting of $\sigma^{(2)}(\theta_{12})$ (dashed line), and the Gaussian fitting of $|a_g(\theta_{12})|^2$ (dotted line).

it happens at $E = 2.5$ eV], similarly to H⁻. Surprisingly, at $E > 5$ eV, the difference between $\gamma(|a_g|^2)$ and $\gamma(\sigma^{(2)})$ became enormous. The origin for this is clear from Fig. 7. The correlation coefficient has a strongly non-Gaussian shape with the two peaks, even at low energy $E = 1$ eV. When the energy decreases, the secondary peak declines and therefore

FIG. 8. (Color online) The Gaussian width *γ* as a function of *E* for the photoionization of He(3 $s¹S$): our results were obtained by the fitting of $\sigma^{(2)}(\theta_{12})$ (thick solid line) and $|a_g(\theta_{12})|^2$ (thin solid line), along with CCC results [\[10\]](#page-6-0).

the distribution turns Gaussian, as follows from Wannier's theory. When the energy increases, the secondary peak grows and becomes larger than the primary peak at $E = 11.3$ eV, as is seen from Figs. $7(b)$ and $7(c)$. Then, naturally, the Gaussian approximation becomes nonapplicable.

In Fig. 8, we show γ as a function of *E* for the photoionization of helium in the $3s¹S$ state. Our results are strongly different from the CCC results [\[10\]](#page-6-0), both in magnitude and in behavior. The general curve shape is similar to that for $2s¹S$, but $\gamma(\sigma^{(2)})$ reaches the local maximum at $E = 1.5$ eV. It is seen from Fig. [9](#page-5-0) that the correlation parameter is strongly non-Gaussian, as for $2s¹S$, but it has three peaks at low energies. When the energy increases, two smaller peaks grow and merge, and the shape of $\sigma^{(2)}(\theta_{12})$ becomes rather complicated at large energies. One can see that the number of $\sigma^{(2)}(\theta_{12})$ peaks at low energies is equal to the number of peaks of the "outer" electron density versus the radius in the initial state of the target. Particularly, it is equal to one for H[−] (Fig. [4\)](#page-3-0), two for He(2*s* ¹*S*) [Fig. 7(a)], and three for He($3s⁻¹S$) [Fig. $9(a)$]. It seems not to be an accidental coincidence, although we still can not propose a rigorous explanation for this effect. If this finding will be confirmed by other examples, it will provide new facilities for qualitative experimental analysis of the target electronic structure using the over-threshold double photoionization by analogy with the (*e,*2*e*) spectroscopy [\[20\]](#page-6-0).

Having established that the local minimum appearance in the $\gamma(E)$ is common for all considered targets with the asymmetrical initial-state configuration, we can proceed to clarifying the origin of this effect. For all targets, the local minima of $\gamma(E)$ are observed at energies not directly proportional to the target's first ionization potential I_1 , but of the order of *I*1. We should note that, despite the absence of a local minimum in the plot for helium in the ground state (Fig. [1\)](#page-2-0), there is a curve bend at about $E = 20$ eV that indicates some change taking place at the energy of the order of *I*1. In the nonsequential double ionization considered here, one of the electrons is ionized at first by the photon impact, and the second electron might be ejected through a sudden change of the atomic potential (the so-called shake-off mechanism), or through the first electron impact (the so-called

FIG. 9. (Color online) The 2DCS as a function of the interelectron angle θ_{12} for the photoionization of He(3*s*¹*S*) for (a) $E = 1$ eV, (b) $E = 5$ eV, and (c) $E = 20$ eV: "exact" TDS results (solid line), Gaussian fitting of $\sigma^{(2)}(\theta_{12})$ (dashed line), and the Gaussian fitting of $|a_g(\theta_{12})|^2$ (dotted line).

final-state scattering or knock-out mechanism) [\[21\]](#page-6-0). If the initial-state configuration is strongly asymmetrical, then the inner-electron momentum density is much broader than that for the outer electron, and the single-ionization cross-section dependence on the ejection energy for the inner electron decreases much slower than for the outer electron. This means

that the process, when the outer electron is ionized first, may give a significant contribution only when *E* is of the order of the outer-electron binding energy, i.e., *I*1. On the other hand, it is obvious that the shake-off mechanism may give a significant contribution only in the case wherein the first ionized electron velocity is much larger than the velocity distribution width for the second one. Indeed, when the velocity of the first ionized electron is comparable to the velocity of the bound electron, then the potential affecting the second electron changes slowly, and the second electron adiabatically comes to the bound state with the same symmetry as its initial state, as per the well-known theorem; hence, its ionization can not proceed. Therefore, when the outer electron is ionized first, the shake-off mechanism is impossible. However, the possibility of the final-state scattering is also extremely small if the outer electron is ionized first because it can not have enough energy to eject the strongly bound inner electron. Consequently, the double ionization is possible only if the inner electron is ionized first. In this case, the shake-off mechanism is significant only at emission energies much larger than the first ionization potential. From the comparison of γ for the double photoionization of He with γ for (*e*,2*e*) on He⁺ in [\[10\]](#page-6-0), it is clear that the angular interelectron correlations are stronger for the shake-off process than for the final-state scattering. To summarize, we can conclude that γ decreases with the energy decreasing for both processes taken individually, and the *γ* increasing at low energies in Figs. [3,](#page-2-0) [6,](#page-3-0) and [8](#page-4-0) results from the "switching off" of the shake-off process. The distinction from He in the ground state is just the sharpness of this switching off because of the narrow momentum spectrum of the outer electron. It may be predicted that, in the double photoionization of targets with I_1 much less than I_2 (like alkalimetal atoms), $\gamma(E)$ should behave similarly to that for H⁻ in Fig. [3.](#page-2-0)

V. CONCLUSION

We calculated using the *ab initio* method the Gaussian width γ dependence on the energy E of electrons in the double photoionization of the negative hydrogen ion H−, the helium in the ground $1s^2$ state, and the $2s^1S$ and $3s^1S$ excited states. For the $He(1s^2)$ photoionization, our results are in perfect agreement with experimental data, but indicate that the well-known Wannier threshold law $\gamma \propto E^{1/4}$ is not correct, even for sufficiently small excess energies of about 0.1 eV. It is shown that the γ dependence on the energy is much better described by the law obtained by Kasansky and Ostrovsky, where the influence of the electrons' deceleration by the nucleus field is properly taken into account. Their law is strongly different from the Wannier threshold law at any values of the excess energy, even at extremely low ones, and, therefore, the Wannier threshold law is meaningless in the interpretation of experimental and theoretical angular distribution data. We have also shown that for all considered targets with strongly asymmetrical initial-state configuration, there is a region of excess energy where derivative of $\gamma(E)$ with respect to *E* is negative. We suppose that this effect is due to a rapid change of the dominating ionization mechanism from shake-off to the less-correlated final-state scattering. Also, it

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was demonstrated that the cross-section dependence on the interelectron energy for these targets is strongly non-Gaussian at low energies and has a number of peaks equal to the number of the initial-state radial nodes, which offer new possibilities for the qualitative analysis of the electronic structure of targets.

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