Scattering of wave packets on atoms in the Born approximation

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It has recently been demonstrated experimentally that 200–300 keV electrons with the unusual spatial profiles can be produced and even focused to a subnanometer scale—namely, electrons carrying nonzero orbital angular momentum and also the so-called Airy beams. Since the wave functions of such electrons do not represent plane waves, the standard Born formula for scattering of them off a potential field is no longer applicable and, hence, needs modification. In the present paper, we address the generic problem of elastic scattering of a wave packet of a fast nonrelativistic particle off a potential field. We obtain simple and convenient formulas for a number of events and an effective cross section in such a scattering, which represent generalization of the Born formula for a case when finite sizes and spatial inhomogeneity of the initial packet should be taken into account. As a benchmark, we consider two simple models corresponding to scattering of a Gaussian wave packet on a Gaussian potential and on a hydrogen atom, and perform a detailed analysis of the effects brought about by the limited sizes of the incident beam and by the finite impact parameter between the potential center and the packet's axis.

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I. INTRODUCTION

Let us consider scattering of a particle beam by a potential field. A real beam has finite sizes and a nonuniform density, but usually in the standard theoretical description of the scattering process the beam is replaced with a plane wave. Such an approach is valid for a number of problems in which distances, essential for calculation of the corresponding cross sections, are considerably smaller than the typical sizes of the beam's inhomogeneity. There are, however, important exclusions.

Thus at e^+e^- and ep colliders, several processes were experimentally investigated in which macroscopically large impact parameters gave an essential contribution to the cross section [1]. These impact parameters may be much larger than the transverse sizes of the colliding bunches, and in this case the standard calculations have to be essentially modified. It is the so-called beam size or MD effect, discovered at the MD detector (the VEPP-4 collider in Novosibirsk; see review in [1]), which leads to the essential reduction of the beam particle losses at modern colliders [2]. Another important example here is the so-called prewave zone effect in electromagnetic radiation by electrons [3], which is of high importance for the beam diagnostic techniques in modern accelerators [4]. Note that these phenomena are directly related to the ultrarelativistic particles.

Recently, several groups have reported on the experimental creation of electrons possessing unusual features—namely, of the so-called "vortex" or "twisted" electrons with a definite value $\hbar m$ of the *orbital angular momentum* (OAM) projection on the beam propagation axis [5,6], including such beams with the orbital quantum number m up to $m = 200$ [7], and also of the so-called Airy electrons [8]. Both of the electron beams produced have nontrivial spatial profiles and, hence, cannot be described with the plane waves; they also resemble corresponding laser beams, which are well known and routinely used in the modern quantum optics—for twisted photons, see a review, e.g., in Refs. [9,10]; for Airy photons see, e.g., Ref. [8] and references therein.

The vortex beams can be manipulated and focused just as the conventional electron bunches, and recently remarkable focusing to a focal spot of less than 0.12 nm in diameter was achieved [11]. It means that wave packets in a form of such electrons could emerge as a new tool in atomic physics; however, while the use of the wave packets instead of plane waves may be usually avoided in the standard approach (see, e.g., Chap. 4.5 in [12]), this seems to be no longer the case for scattering problems with the twisted electrons and photons, as well as with the Airy ones. Indeed, the use of the pure Bessel (non-normalizable) states of twisted electrons was shown to be inconsistent with the conservation law of the OAM in a $2 \to 2$ scattering, and only the formalism of the well-normalized wave packets removes this difficulty [13]. Thus these new quantum states of particles represent another important example of the situation where the standard calculation procedure of scattering has to be essentially modified. For the 200–300 keV electrons realized so far, it is the Born formula that needs some generalization for the case when the incoming particle is described with a wave packet rather than with a plane wave.

In the present paper, we address the generic problem of how to describe elastic scattering of the wave packet of fast nonrelativistic particles off a potential field of an atom and of the atomic structures. One of the first atomic processes with the twisted electrons—a radiative capture of twisted electrons by the bare ions with the emission of a photon—has recently been studied theoretically in the paper [14]. Other recent theoretical investigations [15–17] treat some important features of such processes but do not address the generic issue of how to calculate the number of scattering events depending on the limited sizes of the incident beam. To approach this goal, we derive a simple and convenient expression for the number of events, which generalizes the well-known Born approximation for the case when the incident beam is a wave packet of a general form. It is especially important that the observed number of events depends on the impact parameter $\mathbf{b}$ between the potential center and the packet axis—an effect that is absent in the standard approach. We also consider an

example when the wave packet is scattered off the randomly distributed potential centers, which is the simplest case from the experimental point of view. For such a setup, we obtain a simple and transparent expression for the cross section averaged over impact parameters.

Then, as a benchmark, we consider two simple models: (1) scattering of a Gaussian wave packet on a Gaussian potential and (2) scattering of the Gaussian wave packet on a hydrogen atom.

A detailed analysis of the angular distributions of final particles is given, and it is shown how the standard Born results could be recovered in the limit of a very wide packet. Special attention is paid to the dependence of these distributions on the impact parameter of the potential center with respect to the packet's axis. Similar analysis for the case when the incident particles represent vortex or Airy electrons will be presented elsewhere.

The structure of the paper is as follows. In the next section we recall the standard Born approximation including the well-known formulas for scattering on the Gaussian potential and on the hydrogen atom. In Sec. III we derive the basic formulas for scattering of a wave packet on a potential field and in Sec. IV we specify the general approach for the case of the Gaussian wave packet and illustrate this case with a detailed examination of the two aforementioned models. Some conclusions are given in Sec. V.

For definiteness, we consider below the central fields $U(r)$ having in mind that the presented method can be applied for the noncentral fields $U(\mathbf{r})$ as well. To simplify the formulas, we use the units with the Planck constant $\hbar = 1$.

II. STANDARD BORN APPROXIMATION

A. Number of events in the standard Born approximation

Let us consider scattering of the nonrelativistic particles (electrons, for definiteness) off a potential field $U(r)$ whose center is located at the coordinate origin. Let the typical radius of this field's action be of the order of a. If the initial and scattered electrons have momenta $\mathbf{p}_i$ and $\mathbf{p}_f$, then the S-matrix element $\langle f|S|i\rangle$ for the transition between plane waves $|i\rangle = |\mathbf{p}_i\rangle$ and $|f\rangle = |\mathbf{p}_f\rangle$ is expressed via the scattering amplitude $f(\varepsilon_i,\theta,\varphi)$ as follows:

$$\langle f|S|i\rangle = (2\pi)^2 i\,\delta(\varepsilon_i-\varepsilon_f)\frac{f(\varepsilon_i,\theta,\varphi)}{m_e},$$
$$\varepsilon_i = \frac{\mathbf{p}_i^2}{2m_e},\quad \varepsilon_f = \frac{\mathbf{p}_f^2}{2m_e}, \tag{1}$$

where θ and φ are the polar and azimuthal scattering angles and m_e is the electron mass. The standard differential cross section of the process equals

$$\frac{d\sigma_{\rm st}}{d\Omega} = |f(\varepsilon_i,\theta,\varphi)|^2, \tag{2}$$

where $d\Omega$ is the solid angle element. The scattering amplitude in the first Born approximation is related to the Fourier transform of the potential field (see, for example, §126 in the text-book [18]):

$$f(\mathbf{q}) = -\frac{m_e}{2\pi}\int U(r)e^{-i\mathbf{q}\cdot\mathbf{r}}d^3r,\quad \mathbf{q} = \mathbf{p}_f - \mathbf{p}_i. \tag{3}$$

In the standard approach there is an implicit assumption that the particle bunch is wide and long and almost uniform on the distances of the order of a, i. e., the bunch density in the region of active forces is $n(\mathbf{r},t) \approx n(\mathbf{0},t)$, and velocities of all electrons are almost equal to each other and directed along the axis z; therefore,

$$\mathbf{p}_i = m_e\mathbf{v}_i = (0,0,p_i).$$

In such a case the number of particles $d\nu$ scattered over the time dt is determined by a product of the standard differential cross section $d\sigma_{\rm st}$ and the current of particles near the coordinate origin for a given time $v_i n(\mathbf{0},t)dt$, while the total number of the scattered particles for the whole time reads [19]

$$\frac{d\nu_{\rm st}}{d\Omega} = L\frac{d\sigma_{\rm st}}{d\Omega} = L|f(\mathbf{q})|^2,\quad L = \int v_i n(\mathbf{0},t)dt. \tag{4}$$

Let the initial state be the plane wave in a large volume $\mathcal{V} = \pi\mathcal{R}^2 l_z$, where $\mathcal{R}$ is the radius and l_z is the longitudinal length of the bunch. The bunch density during the large time $\Delta t = l_z/v_i$ is almost constant and equals $n(\mathbf{r},t) = N_e/\mathcal{V}$; therefore,

$$L = \frac{N_e}{\mathcal{V}}l_z = \frac{N_e}{\pi\mathcal{R}^2}. \tag{5}$$

Usually, the change of the transverse beam sizes during the scattering can be neglected and the bunch density depends on the time as $n(\mathbf{r},t) = n(\mathbf{r}_\perp, z - v_i t)$. If we define *the transverse density*

$$n_{\rm tr}(\mathbf{r}_\perp) = \int n(\mathbf{r},t)dz, \tag{6}$$

then quantity L coincides with the transverse density at the coordinate origin,

$$L = n_{\rm tr}(\mathbf{r}_\perp = \mathbf{0}). \tag{7}$$

Let us recall two important examples (see, for example, problems to Sec, 126 in the textbook in [18]).

B. Gaussian potential

The Gaussian potential has the form

$$U(r) = V\,e^{-r^2/(2a)^2}. \tag{8}$$

If electrons are fast ($p_i a \gg 1$) and the condition $V \ll p_i/(m_e a)$ is satisfied, then the Born amplitude equals

$$f(\mathbf{q}) = f_0 e^{-(qa)^2},\quad f_0 = -4\sqrt{\pi}m_e V a^3. \tag{9}$$

The total cross section is determined by the small angle region $\theta \lesssim 1/(p_i a)$ and reads

$$\sigma_{\rm st} = \frac{\pi f_0^2}{2a^2 p_i^2}. \tag{10}$$

C. Hydrogen atom in the ground state

The scattering of fast electrons on the hydrogen atom in the ground state is directly related to the scattering on the potential field of the form (see [18], problem 2 to Sec. 36)

$$U(r) = -\frac{e^2}{r}\left(1+\frac{r}{a}\right)e^{-2r/a}, \tag{11}$$

where e is the proton charge and $a = 1/(m_e e^2)$ is the Bohr radius. The Born approximation for fast electrons ($p_i a \gg 1$) is valid if $m_e e^2 \ll p_i$, so the scattering amplitude is equal to

$$f(\mathbf{q}) = \frac{a}{2}\left(\frac{1}{1+(qa/2)^2} + \frac{1}{(1+(qa/2)^2)^2}\right), \tag{12}$$

and the total cross section is

$$\sigma_{\rm st} = \frac{7\pi}{3p_i^2}. \tag{13}$$

III. SCATTERING OF A WAVE PACKET OFF A POTENTIAL FIELD

A. Basic formulas

In this section we follow the approach developed in Sec. 4.1 of the paper in [1]. The initial state of incoming electrons is given by the wave packet of the generic form

$$\int |\mathbf{k}\rangle \Phi(\mathbf{k}) \frac{d^3k}{(2\pi)^{3/2}}, \tag{14}$$

where the packet's wave function in the momentum space $\Phi(\mathbf{k})$ is normalized by the condition

$$\int |\Phi(\mathbf{k})|^2 d^3k = 1. \tag{15}$$

As a consequence, the probability amplitude for transition from this initial state to the final plane-wave state $|\mathbf{p}_f\rangle$ is given by the convolution

$$\begin{aligned} A &= \int \langle \mathbf{p}_f | S | \mathbf{k}\rangle \Phi(\mathbf{k}) \frac{d^3k}{(2\pi)^{3/2}} \\ &= \sqrt{2\pi} i \int \delta(\varepsilon - \varepsilon_f) f(\mathbf{p}_f - \mathbf{k}) \Phi(\mathbf{k}) \frac{d^3k}{m_e}, \\ \varepsilon &= \frac{\mathbf{k}^2}{2m_e}, \end{aligned} \tag{16}$$

while the number of scattered particles equals

$$dv = N_e A A^* \frac{d^3 p_f}{(2\pi)^3}, \tag{17}$$

where N_e is the number of electrons in the initial packet and

$$\begin{aligned} A^* &= -\sqrt{2\pi} i \int \delta(\varepsilon' - \varepsilon_f) f^*(\mathbf{p}_f - \mathbf{k}') \Phi^*(\mathbf{k}') \frac{d^3k'}{m_e}, \\ \varepsilon' &= \frac{(\mathbf{k}')^2}{2m_e}. \end{aligned} \tag{18}$$

Taking into account that $d^3 p_f = p_f^2 dp_f d\Omega$, one can perform integration over the longitudinal momenta k_z and k'_z using the δ functions and obtain

$$\begin{aligned} \frac{dv}{d\Omega} = N_e \int & f(\mathbf{p}_f - \mathbf{k}) \Phi(\mathbf{k}) f^*(\mathbf{p}_f - \mathbf{k}') \\ & \times \Phi^*(\mathbf{k}') \frac{p_f^2}{\tilde{k}_z \tilde{k}'_z} dp_f \frac{d^2k_\perp}{2\pi} \frac{d^2k'_\perp}{2\pi}, \end{aligned} \tag{19}$$

where

$$\begin{aligned} \mathbf{k} &= \left(\mathbf{k}_\perp, \tilde{k}_z = \sqrt{p_f^2 - k_\perp^2}\right), \\ \mathbf{k}' &= \left(\mathbf{k}'_\perp, \tilde{k}'_z = \sqrt{p_f^2 - (k'_\perp)^2}\right). \end{aligned} \tag{20}$$

As the next step we simplify this expression using several natural assumptions. We assume that the wave packets considered have an axial symmetry; therefore, their averaged transverse momentum is zero, $\langle \mathbf{k}_\perp \rangle = \mathbf{0}$, their averaged momentum is

$$\langle \mathbf{k} \rangle = \mathbf{p}_i = m_e \mathbf{v}_i = (0,0,p_i), \tag{21}$$

but the averaged absolute value of the transverse momentum is nonzero,

$$\langle k_\perp \rangle = \varkappa_0 = p_i \tan\theta_k, \tag{22}$$

Here we introduce the angle θ_k, which is an important parameter for the twisted state and usually is called *the conical or opening angle* (see, for example, Refs. [14,16]). The packet axis can be shifted in the transverse xy plane by a distance (an impact parameter) b. Below we often choose the x axis along this shift—in this case $\mathbf{b} = (b,0,0)$, the azimuthal angle φ coincides with the angle between vectors $(\mathbf{p}_f)_\perp$ and $\mathbf{b}$, and the azimuthal angle φ_k coincides with the one between vectors $\mathbf{k}_\perp$ and $\mathbf{b}$.

We assume that the packet's wave function in the momentum space can be presented as a product of wave functions corresponding to the transverse and longitudinal motions (and this factorization conserves in time):

$$\Phi(\mathbf{k}) = \Phi_{\rm tr}(\mathbf{k}_\perp) \Phi_{\rm long}(k_z). \tag{23}$$

Then let these wave functions have the dispersions $\Delta k_x = \Delta k_y \sim 1/\sigma_\perp$, $\Delta k_z \sim 1/\sigma_z$, where $\sigma_\perp$ and σ_z are the transverse and longitudinal averaged sizes of the electron packet. We assume further that these dispersions are small compared to the longitudinal momentum:

$$\Delta k_x = \Delta k_y \sim 1/\sigma_\perp \ll p_i, \quad \Delta k_z \sim 1/\sigma_z \ll p_i. \tag{24}$$

From the experimental point of view, it is interesting to consider a case when the packet's length σ_z is larger than the radius of the field action a, but still small enough to provide such a situation that during the collision time $t_{\rm col} \sim \sigma_z/v_z = m_e \sigma_z/p_i$ the wave packet does not spread essentially in the transverse plane. It means that the collision time has to be considerably smaller than the diffraction time $t_{\rm dif} \sim \sigma_\perp/v_\perp = m_e \sigma_\perp/\varkappa_0$. Therefore, below we assume that

$$a \ll \sigma_z \ll \sigma_\perp \frac{p_i}{\varkappa_0}. \tag{25}$$

For further integration over p_f or $\tilde{k}_z = \sqrt{p_f^2 - k_\perp^2}$ we take into account the following properties of functions under the integral. The amplitude $f(\mathbf{p}_f - \mathbf{k})$ is concentrated near the value $\tilde{k}_z = (\mathbf{p}_f)_z = p_f \cos\theta$ with the dispersion $\sim 1/a$, while the function $\Phi_{\rm long}(\tilde{k}_z)$ is concentrated near the point $\tilde{k}_z = p_i$ with the dispersion $\sim 1/\sigma_z$, which is considerably smaller than $1/a$. Finally, we take into account that the quantities $\tilde{k}_z$ and $\tilde{k}'_z$ depend on $k_\perp$ and $k'_\perp$ but the corresponding variations are

small, for example,

$$|\delta\tilde{k}_z| = \left|\delta\sqrt{p_f^2 - k_\perp^2}\right| \sim \frac{\varkappa_0 \delta k_\perp}{p_i} \tag{26}$$

$$\lesssim \frac{\varkappa_0}{\sigma_\perp p_i} \ll \frac{1}{\sigma_z} \sim \Delta k_z \tag{27}$$

due to the inequality (25). Therefore, we can take the amplitudes $f(\mathbf{p}_f - \mathbf{k})f^*(\mathbf{p}_f - \mathbf{k}')$ out of the integral over p_f in the form $f(\mathbf{p}_f - \mathbf{p}_i - \mathbf{k}_\perp)f^*(\mathbf{p}_f - \mathbf{p}_i - \mathbf{k}'_\perp)$ with $\mathbf{p}_i$ given in Eq. (21).

The rest integral over p_f can be evaluated as follows:

$$\int \Phi_{\text{long}}(\tilde{k}_z)\Phi^*_{\text{long}}(\tilde{k}'_z)\frac{p_f^2}{\tilde{k}_z\tilde{k}'_z}dp_f = \int |\Phi_{\text{long}}(\tilde{k}_z)|^2 \frac{p_f}{\tilde{k}_z}d\tilde{k}_z = \frac{1}{\cos\theta_k}. \tag{28}$$

As a result, we obtain the basic expression

$$\frac{d\nu}{d\Omega} = \frac{N_e}{\cos\theta_k}|F(\mathbf{Q})|^2, \qquad F(\mathbf{Q}) = \int f(\mathbf{Q} - \mathbf{k}_\perp)\Phi_{\text{tr}}(\mathbf{k}_\perp)\frac{d^2k_\perp}{2\pi}, \tag{29}$$

where $\mathbf{Q}$ is

$$\mathbf{Q} = \mathbf{p}_f - \mathbf{p}_i = (\mathbf{Q}_\perp, Q_z),$$
$$\mathbf{Q}_\perp = (\mathbf{p}_f)_\perp = p_f(\sin\theta\ \cos\varphi, \sin\theta\ \sin\varphi, 0), \tag{30}$$
$$Q_z = p_f\cos\theta - p_i, \quad p_f = \sqrt{p_i^2 + \varkappa_0^2}.$$

Let us stress that the formula (29) is valid only under the condition (25)—in other words, this approximation is inapplicable for too small values of $\sigma_\perp$. Besides, we would like to note that in order to obtain this formula we have used a *nonmonochromatic* initial packet. Moreover, in the final state we integrate over the plane waves with the different energies which are detected in the solid angle $d\Omega$. Our final result (29) includes the Born scattering amplitude $f(\mathbf{p}_f - \mathbf{p}_i - \mathbf{k}_\perp)$ in which the initial plane wave has the momentum $\langle\mathbf{k}\rangle + \mathbf{k}_\perp = \mathbf{p}_i + \mathbf{k}_\perp$, while the final plane wave has the momentum $\mathbf{p}_f$ with $|\mathbf{p}_f| = \sqrt{p_i^2 + \langle k_\perp\rangle^2} = \sqrt{p_i^2 + \varkappa_0^2}$.

Below another representation for the integral $F(\mathbf{Q})$ will be useful. It can be obtained if we substitute the evident form of the scattering amplitude from (3) into Eq. (29):

$$F(\mathbf{Q}) = -\frac{m_e}{2\pi}\int U(r)\Psi_{\text{tr}}(\mathbf{r}_\perp)e^{-i\mathbf{Q}\mathbf{r}}d^3r, \tag{31}$$

where

$$\Psi_{\text{tr}}(\mathbf{r}_\perp) = \int \Phi_{\text{tr}}(\mathbf{k}_\perp)e^{i\mathbf{k}_\perp\mathbf{r}_\perp}\frac{d^2k_\perp}{2\pi}. \tag{32}$$

Let us recall that in the standard approach the angular distribution of scattered particles is determined by the scattering amplitude $f(\mathbf{q})$ proportional to the Fourier transform of the potential field $U(r)$ [see Eq. (3)]. The quantity $F(\mathbf{Q})$ plays the same role for the scattering of the wave packet, which is the Fourier transform of the product of functions $U(r)\,\Psi_{\text{tr}}(\mathbf{r}_\perp)$. From here one can draw several qualitative conclusions related to the angular distributions of the scattered electrons (see Sec. IV A below).

B. Averaging over impact parameters

Let the potential centers be randomly distributed inside a large disk of the radius $\mathcal{R} \gg a, \sigma_\perp$. In this case the averaged cross section $d\bar{\sigma}$ is obtained after integrating the number of events over all the impact parameters $\mathbf{b}$ and dividing the result obtained by the total number of particles in the packet:

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{1}{N_e}\int \frac{d\nu}{d\Omega}d^2b, \tag{33}$$

where $d\nu/d\Omega$ is given by Eq. (29).

If the packet axis is shifted in the transverse plane by a distance $\mathbf{b}$ from the potential center, the corresponding wave function in the momentum representation can be written as

$$\Phi_{\text{tr}}(\mathbf{k}_\perp) = a(\mathbf{k}_\perp)e^{-i\mathbf{k}_\perp\mathbf{b}}, \tag{34}$$

where the function $a(\mathbf{k}_\perp)$ corresponds to a nonshifted packet. Therefore, the averaged cross section is proportional to the integral

$$I_{\text{av}} = \int F(\mathbf{Q})F^*(\mathbf{Q})d^2b, \tag{35}$$

where

$$F(\mathbf{Q}) = \int f(\mathbf{Q} - \mathbf{k}_\perp)a(\mathbf{k}_\perp)e^{-i\mathbf{k}_\perp\mathbf{b}}\frac{d^2k_\perp}{2\pi}, \qquad F^*(\mathbf{Q}) = \int f^*(\mathbf{Q} - \mathbf{k}'_\perp)a^*(\mathbf{k}'_\perp)e^{i\mathbf{k}'_\perp\mathbf{b}}\frac{d^2k'_\perp}{2\pi}. \tag{36}$$

After the trivial integration over $\mathbf{b}$ and $\mathbf{k}'_\perp$, we obtain

$$I_{\text{av}} = \int |f(\mathbf{Q} - \mathbf{k}_\perp)|^2|\Phi_{\text{tr}}(\mathbf{k}_\perp)|^2d^2k_\perp, \tag{37}$$

and, therefore,

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{1}{\cos\theta_k}\int |f(\mathbf{Q} - \mathbf{k}_\perp)|^2 dW(\mathbf{k}_\perp), \qquad dW(\mathbf{k}_\perp) = |\Phi_{\text{tr}}(\mathbf{k}_\perp)|^2d^2k_\perp. \tag{38}$$

This expression can be interpreted as averaging of the standard Born cross section $d\sigma_{\text{st}}/d\Omega = |f(\mathbf{Q} - \mathbf{k}_\perp)|^2$ with the shifted momentum transfer $\mathbf{q} \to \mathbf{Q} - \mathbf{k}_\perp$ over probability $dW(\mathbf{k}_\perp)$ to have such a shift in the initial wave packet.

IV. SCATTERING OF A GAUSSIAN WAVE PACKET

In this section we discuss some general properties of the Gaussian wave packets and derive the basic formulas for the models described in Sec. II. The equations obtained will be used for calculating the features of these models.

A. General properties

Let the initial beam be the simplest azimuthally symmetric Gaussian wave packet whose transverse wave function in the momentum representation is

$$\Phi_{\text{tr}}(\mathbf{k}_\perp) = \frac{e^{-(\mathbf{k}_\perp\sigma_\perp)^2 - i\mathbf{k}_\perp\mathbf{b}}}{\sqrt{\pi/(2\sigma_\perp^2)}}. \tag{39}$$

Therefore, the dispersion is $\Delta k_x = \Delta k_y = 1/(2\sigma_\perp)$ and the transverse momentum is found as

$$\langle \mathbf{k}_\perp \rangle = 0, \quad \langle k_\perp \rangle = \varkappa_0 = \frac{\sqrt{\pi}}{2\sqrt{2}\sigma_\perp} \approx \frac{0.63}{\sigma_\perp}. \tag{40}$$

Assuming that the distribution in Eq. (39) is sharp and taking into account the inequality (24), we can put below for simplicity

$$\theta_k = 0$$

for the Gauusian wave packet. The coordinate wave function reads

$$\Psi_{\rm tr}(\mathbf{r}_\perp,t) = \int \Phi_{\rm tr}(\mathbf{k}_\perp) e^{i[\mathbf{k}_\perp \mathbf{r}_\perp - \mathbf{k}_\perp^2 t/(2m_e)]} \frac{d^2k_\perp}{2\pi} \tag{41}$$

and the transverse density equals

$$n_{\rm tr}(\mathbf{r}_\perp,t) = N_e |\Psi_{\rm tr}(\mathbf{r}_\perp,t)|^2 = \frac{N_e}{2\pi\sigma_\perp^2(t)} e^{-(\mathbf{r}_\perp - \mathbf{b})^2/[2\sigma_\perp^2(t)]}. \tag{42}$$

For such a packet, $\langle \mathbf{r}_\perp \rangle = \mathbf{b}$ and the dispersions are

$$\Delta x = \Delta y = \sigma_\perp(t) = \sqrt{\sigma_\perp^2 + \left(\frac{t}{2\sigma_\perp m_e}\right)^2}. \tag{43}$$

We use the approximation (25), which implies that during the collision time the transverse dispersion $\sigma_\perp(t)$ does not differ much from $\sigma_\perp$. In this case, the function

$$\Psi_{\rm tr}(\mathbf{r}_\perp,t) \approx \Psi_{\rm tr}(\mathbf{r}_\perp) = \int \Phi_{\rm tr}(\mathbf{k}_\perp) e^{i\mathbf{k}_\perp \mathbf{r}_\perp} \frac{d^2k_\perp}{2\pi} \tag{44}$$

and the quantity L from (7) (at $b = 0$) becomes equal to

$$L = n_{\rm tr}(\mathbf{0}) = N_e \left| \int \Phi_{\rm tr}(\mathbf{k}_\perp) \frac{d^2k_\perp}{2\pi} \right|^2 = \frac{N_e}{2\pi\sigma_\perp^2} \tag{45}$$

[compare this expression with (5)].

If the Gaussian packet is wide, $\sigma_\perp \gg a$, the behavior of the function $U(r)\Psi_{\rm tr}(\mathbf{r}_\perp)$ in the essential region of integration in Eq. (31) is almost the same as the one of the potential field $U(r)$. In this case the function $F(\mathbf{Q})$ has almost the same behavior as the standard Born amplitude $f(\mathbf{q})$. With the decrease of $\sigma_\perp$, behavior of these two functions becomes more and more different. For example, decrease of the function $U(r)\,\Psi_{\rm tr}(\mathbf{r}_\perp)$ with the growth of r becomes sharper and, therefore, in the function $F(\mathbf{Q})$ the role of the larger values of Q, compared to the standard Born amplitude $f(\mathbf{q})$, increases. As a result, the angular distributions become wider compared to the standard case.

Let us show how the standard result follows from Eq. (29). The standard case corresponds to a wide packet which has the distribution over $\mathbf{k}_\perp$ concentrated in the narrow region near $\langle k_\perp \rangle = \varkappa_0 \approx 0$. Therefore, in the amplitude $f(\mathbf{Q} - \mathbf{k}_\perp)$ we can put $\mathbf{k}_\perp = \mathbf{0}$ and take this amplitude out of the integral over $\mathbf{k}_\perp$ in Eq. (29). After that this equation becomes of the form

$$\frac{dv}{d\Omega} = |f(\mathbf{q})|^2 N_e \left| \int \Phi_{\rm tr}(\mathbf{k}_\perp) \frac{d^2k_\perp}{2\pi} \right|^2, \tag{46}$$

which coincides with the standard result (4) for the number of the scattered particles if we take into account the relation (45).

Analogously, the averaged cross section for a wide wave packet coincides with the standard cross section:

$$\frac{d\bar{\sigma}}{d\Omega} = |f(\mathbf{q})|^2 \int dW(\mathbf{k}_\perp) = |f(\mathbf{q})|^2 = \frac{d\sigma_{\rm st}}{d\Omega} \quad \text{at } \sigma_\perp \gg a. \tag{47}$$

B. Model 1—scattering of the Gaussian wave packet on the Gaussian potential

For the potential field of the Gaussian form (8), the integral $F(\mathbf{Q})$ in Eq. (29) is calculated analytically

$$F(\mathbf{Q}) = B \frac{e^{(Q_\perp a)^2/(1+\sigma_\perp^2/a^2)}}{1 + a^2/\sigma_\perp^2} \frac{f(\mathbf{Q})}{\sqrt{2\pi}\sigma_\perp} e^{-i\beta}, \quad Q_\perp = p_f \sin\theta, \tag{48}$$

where

$$B = e^{-b^2/[4(\sigma_\perp^2 + a^2)]}, \quad \beta = \frac{\mathbf{Q}_\perp \mathbf{b}}{1 + \sigma_\perp^2/a^2}. \tag{49}$$

The final results for the number of events and for the averaged cross section for a wide beam have simple analytical forms:

$$\begin{aligned} \frac{dv}{d\Omega} &= B^2 \frac{e^{2(Q_\perp a)^2/(1+\sigma_\perp^2/a^2)}}{(1 + a^2/\sigma_\perp^2)^2} \frac{dv_{\rm st}}{d\Omega}, \\ \frac{dv_{\rm st}}{d\Omega} &= L \frac{d\sigma_{\rm st}}{d\Omega}, \quad L = \frac{N_e}{2\pi\sigma_\perp^2}, \\ \frac{d\bar{\sigma}}{d\Omega} &= \frac{e^{2(Q_\perp a)^2/(1+\sigma_\perp^2/a^2)}}{(1 + a^2/\sigma_\perp^2)} \frac{d\sigma_{\rm st}}{d\Omega}. \end{aligned} \tag{50}$$

It is easy to see from this expression that for a wide beam (at $\sigma_\perp \gg a,b$) we get the standard results.

C. Models 2—scattering of the Gaussian wave packet on the hydrogen atom in the ground state

The potential field of the hydrogen atom in the ground state is given by Eq. (11). In this case the integral $F(\mathbf{Q})$ in Eq. (29) can be calculated using the substitution

$$\begin{aligned} f(\mathbf{Q} - \mathbf{k}_\perp) &= f_0 \left(\frac{1}{z} + \frac{1}{z^2} \right) = f_0 \int_0^\infty (1 + x) e^{-xz} dx, \\ z &= 1 + \frac{1}{4}(\mathbf{Q} - \mathbf{k}_\perp)^2 a^2 \end{aligned} \tag{51}$$

and further simple integration over $\mathbf{k}_\perp$. As a result, the differential number of events is expressed via a one-fold integral over the variable x:

$$\frac{dv}{d\Omega} = L f_0^2 \left| \int_0^\infty e^{-x g_0 - i g_1 b \cos\varphi - g_2 b^2} \frac{1 + x}{1 + x/s} dx \right|^2, \tag{52}$$

$$\begin{aligned} L &= \frac{N_e}{2\pi\sigma_\perp^2}, \quad s = \frac{4\sigma_\perp^2}{a^2}, \\ g_0 &= 1 + \frac{(Q_\perp a)^2}{4(1 + x/s)} + \frac{(Q_z a)^2}{4}, \\ g_1 &= \frac{x}{x + s} Q_\perp, \quad g_2 = \frac{1}{(x + s)a^2}. \end{aligned} \tag{53}$$

It is easy to check that Eq. (52) does not change under the replacement $\varphi \to \pi + \varphi$. It means that the number of events is symmetric with respect to the angle $\varphi = \pi$.

In a similar way, the averaged cross section (38) can be calculated using the substitution

$$|f(\mathbf{Q}-\mathbf{k}_\perp)|^2 = f_0^2\left(\frac{1}{z^2}+\frac{2}{z^3}+\frac{1}{z^4}\right) = f_0^2\int_0^\infty\left(x+x^2+\frac{1}{6}x^3\right)e^{-xz}dx \qquad (54)$$

and further simple integration over $\mathbf{k}_\perp$, which results in the following expression:

$$\frac{d\bar{\sigma}}{d\Omega} = f_0^2\int_0^\infty e^{-xg}\frac{x+x^2+(x^3/6)}{1+x/(2s)}dx, \quad g = 1+\frac{(Q_\perp a)^2}{4[1+x/(2s)]}+\frac{(Q_z a)^2}{4}. \qquad (55)$$

In the limiting case of the wide packet (at $\sigma_\perp \gg a,b$) we obtain

$$g_0 = g = 1+(qa/2)^2, \quad g_1 = g_2 = 0, \quad \frac{d\nu}{d\Omega} = Lf_0^2\left(\frac{1}{g}+\frac{1}{g^2}\right)^2, \quad \frac{d\bar{\sigma}}{d\Omega} = f_0^2\left(\frac{1}{g}+\frac{1}{g^2}\right)^2, \qquad (56)$$

i.e., the standard results.

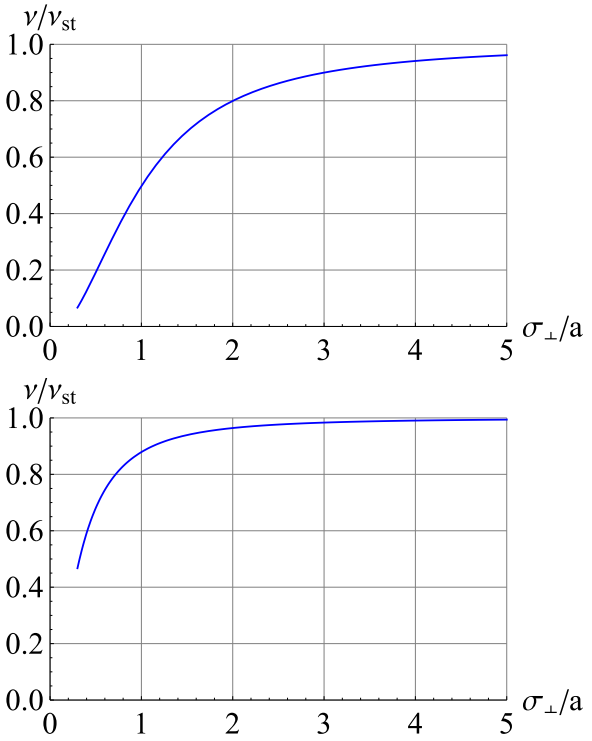

FIG. 1. (Color online) (*On top*) Scattering of the Gaussian packet (39) on the Gaussian potential. Relative number of events vs $\sigma_\perp/a$ at $b = 0$. (*Below*) The same, but for the scattering on the hydrogen atom.

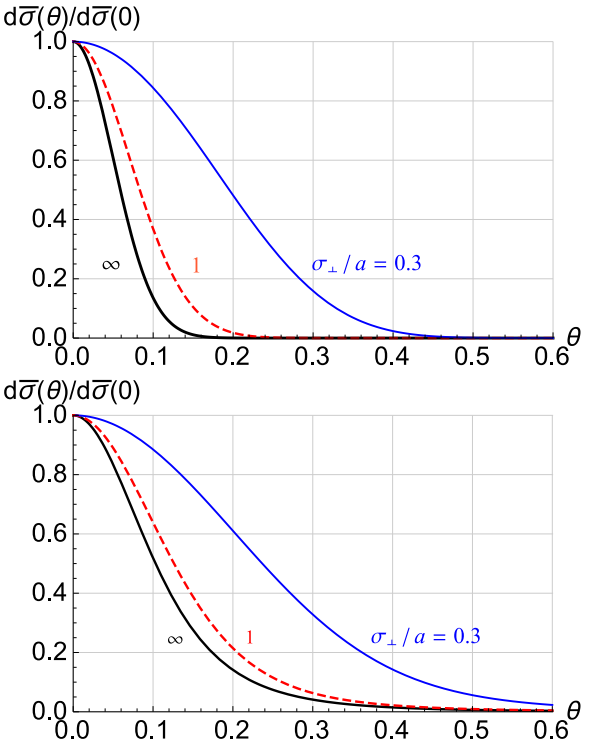

FIG. 2. (Color online) (*On top*) Scattering of the Gaussian packet (39) on the Gaussian potential. Relative differential averaged cross section (57) for $\sigma_\perp/a = 0.3$, 1, and ∞ (from top to bottom). (*Below*) The same, but for scattering on the hydrogen atom.

D. Comparison of models

In this section we compare scattering of the Gaussian packet on the Gaussian potential and on the hydrogen atom in the ground state. All figures in this subsection are calculated for $p_i a = p_f a = 10$; for scattering on the hydrogen atom this corresponds to the energy $\varepsilon_i = 1.36$ keV.

1. Central collision: b = 0

Let us consider first the case of the central collision, when the impact parameter $b = 0$. One may ask what happens to the number of events ν with the decrease of the transverse size of

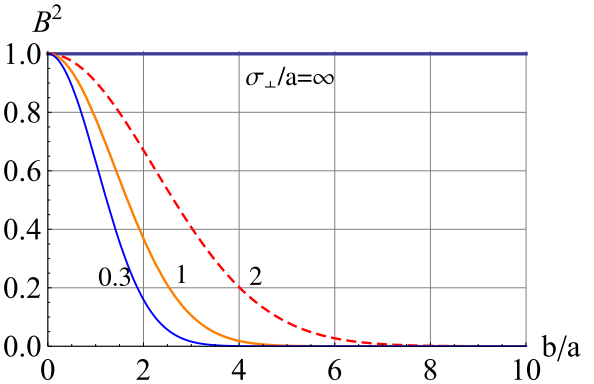

FIG. 3. (Color online) Scattering of the Gaussian packet (39) on the Gaussian potential. The function B^2 from Eq. (49) vs b/a at $\sigma_\perp/a = \infty$, 2, 1, and 0.3 .

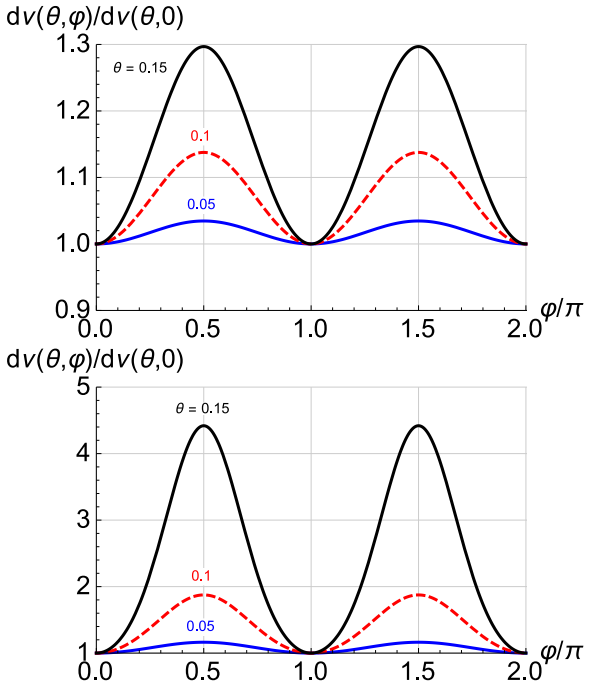

FIG. 4. (Color online) (*On top*) Scattering of the Gaussian packet (39) with $\sigma_\perp = a$ on the hydrogen atom in the ground state. Relative differential number of events vs azimuthal angle φ at $b = 2.5a$ and $\theta = 0.15$, 0.1, and 0.05. (*Below*) The same, but for $b = 5a$.

the bunch $\sigma_\perp$. It is clearly seen from Fig. 1 that the ratio of ν to the standard number of events $\nu_{\rm st}$ decreases.

On the contrary, the angular distributions, $d\nu(\theta)/d\Omega$ or $d\bar{\sigma}(\theta)/d\Omega$, over the polar angle θ become wider with the decrease of $\sigma_\perp$ (just as we expected—see Sec. IV A). This feature is illustrated with Fig. 2, which presents the relative angular distributions

$$\frac{d\bar{\sigma}(\theta)/d\Omega}{d\bar{\sigma}(0)/d\Omega} \tag{57}$$

for $\sigma_\perp/a = \infty$, 1, and 0.3. The physical picture is that with the decrease of $\sigma_\perp$, the density of the particle current increases in the vicinity of the potential center and more particles are scattered at larger angles, but probability of such scattering becomes smaller; the analytical expression (50) supports such an interpretation.

2. *Noncentral collision:* $\mathbf{b} \neq \mathbf{0}$

The number of events drops quickly with the increase of the impact parameter b. It is clearly seen for the model 1 where all the dependence on b is determined by the function $B^2(b)$ [see Eqs. (49) and (50)]. This function is presented in Fig. 3 for $\sigma_\perp/a = \infty$, 2, 1, and 0.3. It is seen that this dependence is absent for the standard cross section (at $\sigma_\perp \gg a,b$). But with the decreasing $\sigma_\perp$, the observed cross section drops more and more quickly with the growth of b.

From the general point of view, we expect that an azimuthal asymmetry should appear in the angular distributions at $b \neq 0$. It is quite interesting to note that for the simplest model 1 this general expectation does not take place. Indeed, even though the quantity $F(\mathbf{Q})$ (48) has the factor $e^{-i\beta}$, which does depend on the azimuthal angle between the vectors $\mathbf{Q}_\perp$ and $\mathbf{b}$, the number of events, being proportional to $|F(\mathbf{Q})|^2$, does not depend on this angle.

In contrast to the model 1, the azimuthal asymmetry reappears in the model 2. For this one at $\sigma_\perp = a$ we present in Fig. 4 the quantity

$$\frac{d\nu(\theta,\varphi)/d\Omega}{d\nu(\theta,0)/d\Omega} \tag{58}$$

for different values of the polar angle $\theta = 0.05$, 0.1, and 0.15. It is seen that the discussed ratio of the cross sections increases considerably at the angles of $\varphi = \pi/2$ and $\varphi = 3\pi/2$ (that is perpendicular to the direction of $\mathbf{b}$) with the growth of the impact parameter.

V. SUMMARY

We derived simple and convenient expressions (29) and (31) for the number of scattering events, which generalizes the well-known Born approximation for the case when the initial beam is a well-normalized wave packet, but not a plane wave. Then we applied the formulas obtained to a couple of benchmark models corresponding to scattering of the Gaussian wave packet on the Gaussian potential as well as on the hydrogen atom, and show how the standard Born results can be recovered in the limit of a very wide incident packet.

The detailed analysis has been performed of how the total number of events and its angular distributions depend on the limited sizes of the incident beam and on the impact parameters between the potential center and the packet's axis. In particular, we have found that the angular distributions of the effective cross section broaden with the decrease of the packet's width—this behavior is somewhat similar to the prewave zone effect in transition radiation; see Ref. [3]. The nonzero impact parameter of the wave packet was shown to lead to azimuthal asymmetry in the angular distributions, but, somewhat unexpectedly, this natural effect is absent in the model of the Gaussian potential.

As a next step, we can apply the obtained formulas to scattering by atoms of such novel quantum states as twisted electrons and the Airy beams. Such an analysis is currently underway and it will be reported in a separate article.

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