

Atomic processes with twisted electrons

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Abstract. The present status of the fully-relativistic nonperturbative calculations of the fundamental atomic processes with twisted electrons is presented. In particular, the elastic (Mott) scattering, the radiative recombination, and for the very first time, the Bremsstrahlung processes are considered. The electron-ion interaction is accounted for in a nonperturbative manner, that allows obtaining reliable results for heavy systems. We investigate the influence of the “twistedness” of the incoming electron on the angular and polarization properties of the emitted electrons and photons for the elastic and inelastic scattering, respectively. It is found that these properties exhibit a strong dependence on the opening angle of the vortex electron beam in all processes considered.

1. Introduction

The electron is called twisted (or vortex) if it possesses a well-defined total angular momentum projection onto the propagation direction. Such particles being the solutions of the free Dirac equation with the imposed cylindrical boundary conditions were predicted theoretically [1] and realized experimentally [2, 3, 4] about a decade ago. From these articles, the extensive investigations dedicated to the creation, detection, and application of twisted electrons have started (see [5, 6, 7] for a review and relevant references). The interest in such particles is caused mainly by the magnitude of their total angular momentum (TAM) projection $\hbar m$. This projection can substantially exceed the one defined solely by the spin angular momentum of the conventional (plane-wave) electrons. Nowadays, the twisted electrons with $m \sim 1000$ can be routinely produced [8]. The magnetic dipole moment $\mu = m\mu_B$ (μ_B is the Bohr magneton) of the electrons with such a high TAM projection is by three orders of magnitude larger than those in the plane-wave case. This fact stimulates investigations of the utility of the twisted electrons for studying various subtle magnetic effects [9] and magnetic properties of the materials [10, 11, 12, 13].

Interaction of twisted electrons with ionic and atomic targets is of particular interest. Indeed, with the growth of TAM projection, the spin-orbit interaction increases thus providing a unique opportunity to get a better insight into the role of the complex interplay between spin and orbital angular momenta in various atomic processes. This fact has stimulated investigations of processes involving ionic (or



atomic) targets and twisted electrons. In [14], the transfer of the orbital angular momentum from an incident vortex beam to the internal motion of the hydrogen electron was studied. The Rutherford potential scattering of electron vortices was investigated in [15]. Matula and co-authors [16] discussed the radiative recombination of twisted beams with bare nuclei into the ground states of corresponding H-like ions. The atom excitation in course of the inelastic electron-vortex-beam scattering was studied in [17]. In [18, 19], the investigation of the beam-size effects in the scattering of the twisted packets by the hydrogen atom was presented. Serbo *et al* [20] examined the Mott scattering of high-energy twisted electrons by neutral atoms whose electrostatic potential was approximated by a sum of three Yukawa potentials. The detailed description of the hydrogen atom ionization by the vortex beam was presented in the recent work by Harris and co-authors [21]. It is worth mentioning that only in [20] the relativistic formalism was utilized meanwhile in other investigations the nonrelativistic approach was used.

All these studies, however, were performed in the framework of the first Born approximation, i.e., the interaction of the twisted electrons with the target potential was taken into account in a perturbative manner. Such approximation is applicable only for the description of low- Z (Z is the nuclear charge number) atomic systems and relatively large projectile velocities. Meanwhile, the largest sensitivity to the “twistedness” is expected in high- Z systems where the spin-orbit interaction is strongly enhanced. To perform an accurate description of the processes with heavy ions and atoms, one needs to account for the interaction of the vortex electron with the target potential nonperturbatively. In [22] the fully-relativistic approach aimed at performing such descriptions was developed. In this formalism, the vortex electron is described by the wave function being the solution of the Dirac equation with the target potential and the twisted-wave asymptotic behavior. As a first application of the developed approach, in [22] the recombination of the vortex electron beams with heavy bare nuclei was described in details. Later, Kosheleva and co-authors [23] applied a similar method for the investigation of the higher-order effects beyond the first Born approximation in the process of the elastic (Mott) scattering of twisted electrons by neutral atoms. Additionally, in this work, the differential cross section and the degree of longitudinal polarization for scattering by such a heavy element as gold ($Z = 79$) were evaluated. We also mention another approach for the description of the twisted electrons in external fields which is based on the Foldy-Wouthuysen representation of the Dirac equation. This approach was successfully applied by Silenko and co-authors [24] to study the twisted electrons in electric and magnetic fields.

Here we apply the formalism developed in [22] for the investigation of the fundamental atomic processes with twisted electrons. In particular, the elastic (Mott) scattering, the radiative recombination, and the Bremsstrahlung processes are considered. It should be noted that the Bremsstrahlung from twisted electrons propagating in the field of ionic or atomic targets has not been examined so far. We pay special attention to the investigation of the influence of the “twistedness” of the incoming electron on the angular and polarization properties of the emitted electrons and photons for the elastic and inelastic scattering, respectively. It is found that these properties exhibit a strong dependence on the opening angle of the vortex electron beam in all processes considered.

2. Basic formalism

Let us start with the brief recall of the main properties of the free twisted electrons which we take here in the form of the Bessel waves. The vortex states are characterized by the following set of quantum numbers: the energy ε , the helicity μ , and the projections of the linear p_z and total angular m momenta onto the propagation direction which is chosen as the z -axis. Twisted electrons also possess a well-defined transversal momentum $\varkappa = \sqrt{\varepsilon^2 - 1 - p_z^2}$ and the so-called opening angle $\theta_p = \arctan(\varkappa/p_z)$. The explicit expression for the wave function of the state with the quantum numbers listed above is given by [20]

$$\psi_{\varkappa m p_z \mu}(\mathbf{r}) = \int d\mathbf{p} \frac{e^{im\varphi_p}}{2\pi p_\perp} \delta(p_\parallel - p_z) \delta(p_\perp - \varkappa) i^{\mu-m} \psi_{\mathbf{p}\mu}(\mathbf{r}). \quad (1)$$

Here p_{\parallel} and p_{\perp} are the longitudinal and perpendicular components of the momentum \mathbf{p} , respectively, and $\psi_{\mathbf{p}\mu}$ is the plane-wave solution of the free Dirac equation

$$\psi_{\mathbf{p}\mu}(\mathbf{r}) = \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{2\varepsilon(2\pi)^3}} u_{\mathbf{p}\mu}, \quad (2)$$

where $u_{\mathbf{p}\mu}$ is the Dirac bispinor [25, 26] which satisfies the normalization condition $u_{\mathbf{p}\mu}^{\dagger} u_{\mathbf{p}\mu'} = 2\varepsilon\delta_{\mu\mu'}$. Equation (1) implies that in the momentum space, the twisted electron can be represented as a coherent superposition of the plane-waves with the linear momenta \mathbf{p} covering the surface of a cone with the opening angle θ_p . Additionally, from equation (1), it is seen that the vortex beam has an inhomogeneous probability distribution and an inhomogeneous flux density. In particular, the flux density equals

$$j_z^{(\text{tw})}(\mathbf{r}) = \psi_{\mathcal{X}mp_z\mu}^{\dagger}(\mathbf{r})\alpha_z\psi_{\mathcal{X}mp_z\mu}(\mathbf{r}) = \frac{p}{\varepsilon(2\pi)^3} \sum_{\sigma} 4\mu\sigma \left[d_{\sigma\mu}^{1/2}(\theta_p) \right]^2 J_{m-\sigma}^2(\mathcal{X}r_{\perp}), \quad (3)$$

where $p = |\mathbf{p}|$, α_z is the z component of the vector of Dirac matrices, $d_{MM'}^J(\theta)$ is the small Wigner matrix [27, 28], J_n is the Bessel function of the first kind [29, 30], and r_{\perp} is the perpendicular component of \mathbf{r} .

Having discussed the basic properties of the free twisted electrons, we proceed to study their scattering (elastic and inelastic) by a single ion. First, we fix the z -axis along the propagation direction of the vortex beam. The position of the ion is given by the impact parameter $\mathbf{b} = (b_x, b_y, 0)$, which defines the relative position of the target and the incident electron. The necessity of this parameter is provided by the inhomogeneity of the probability flux density (3) of the vortex beam. To describe the scattering of the vortex beam by heavy ions accurately, one needs to account for the electron-atom interaction nonperturbatively. It can be performed via the construction of the wave function of the twisted electron as the solution of the Dirac equation in the external field of the ionic target with the following asymptotics [31]

$$\Psi_{\mathcal{X}mp_z\mu}^{(+)}(\mathbf{r} + \mathbf{b}) \xrightarrow{r \rightarrow \infty} \psi_{\mathcal{X}mp_z\mu}(\mathbf{r} + \mathbf{b}) + G_{m\mu, \mathbf{b}}^{(\text{tw})}(\theta_p, \mathbf{n}) \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{r}. \quad (4)$$

Here $G^{(\text{tw})}$ is the bispinor amplitude and the transformed coordinate system $\mathbf{r} - \mathbf{b} \rightarrow \mathbf{r}$ (being convenient for practical calculations) is used. The wave function (4) is given by [22]

$$\Psi_{\mathcal{X}mp_z\mu}^{(+)}(\mathbf{r} + \mathbf{b}) = \int d\mathbf{p} \frac{e^{im\varphi_p}}{2\pi p_{\perp}} \delta(p_{\parallel} - p_z) \delta(p_{\perp} - \mathcal{X}) i^{\mu-m} e^{i\mathbf{p}\cdot\mathbf{b}} \Psi_{\mathbf{p}\mu}^{(+)}(\mathbf{r}), \quad (5)$$

where $\Psi_{\mathbf{p}\mu}^{(+)}$ describes the conventional (asymptotically plane-wave) electron propagating in the ionic target potential. The explicit form of this wave function can be found, e.g., in [26, 32, 33]. Utilizing (5) one can connect the amplitude of the twisted electron scattering with the plane-wave one as follows

$$\tau_{\mathcal{X}mp_z\mu}^{(\text{tw})}(\mathbf{b}) = \int \frac{e^{im\varphi_p}}{2\pi p_{\perp}} \delta(p_{\parallel} - p_z) \delta(p_{\perp} - \mathcal{X}) i^{\mu-m} e^{i\mathbf{p}\cdot\mathbf{b}} \tau_{\mathbf{p}\mu}^{(\text{pl})} d\mathbf{p}. \quad (6)$$

This amplitude accounts for the electron-ion interaction to all orders and describes the scattering process uniquely. Thus, the theoretical description is regarded as complete.

The process of the scattering of the vortex beam by a single ion is challenging for the experimental realization. Here, therefore, a more realistic scenario of the scattering by an infinitely extended (macroscopic) target is considered. We describe this target as an incoherent superposition of ions being randomly and homogeneously distributed. The differential cross section for this case is given by [20]:

$$d\sigma^{(\text{tw})} = \int \frac{d\mathbf{b}}{\pi R^2} \left| \tau_{\mathcal{X}mp_z\mu}^{(\text{tw})}(\mathbf{b}) \right|^2 = \frac{1}{\cos\theta} \int \frac{d\varphi_p}{2\pi} d\sigma^{(\text{pl})}(\hat{\mathbf{p}}), \quad (7)$$

where (πR^2) stands for the cross section area (R is the radius of the cylindrical box) and the volumes of the phase spaces are omitted for brevity. The integrand in this expression designates the differential cross section for the scattering of the plane-wave electron incoming along $\hat{\mathbf{p}} = \mathbf{p}/|\mathbf{p}|$ direction. From equation (7) it is seen that the cross section for the scattering of the twisted electrons by the macroscopic target does not depend on the TAM projection m . It is worth mentioning that this dependence is restored if the incident electron is chosen as a superposition of two (or more) vortex states with different TAM projections [34, 35, 16, 22].

3. Results and discussions

We apply the approach which is described above for the investigation of the fundamental atomic processes with the twisted electrons. In particular, the elastic (Mott) scattering, the radiative recombination, and the Bremsstrahlung processes are studied. Here we restrict ourselves to the consideration of the scattering of 100 keV twisted electrons by the macroscopic target consisting of lead ($Z = 82$) nuclei. Additionally, we consider that the electrons and photons emitted in the course of the processes under investigation are asymptotically described by the plane waves. This assumption corresponds to the fact that in experiments the detectors of the conventional (plane-wave) particles are mostly utilized.

3.1. Elastic (Mott) scattering of twisted electrons

We start with the elastic (Mott) scattering of the twisted electrons. For this process, equation (7) takes the following form

$$\frac{d\sigma_{\mu_f\mu_i}^{(tw)}}{d\Omega_f} = \frac{1}{\cos\theta_p} \int \frac{d\varphi_p}{2\pi} \frac{d\sigma_{\mu_f\mu_i}^{(pl)}}{d\Omega_f}(\hat{\mathbf{p}}), \quad (8)$$

where the solid angle of the emitted electron Ω_f is defined by the azimuthal φ_f and polar θ_f angles, μ_f and μ_i are the helicities of the initial and final electron states, respectively. The explicit expression for the differential cross section of the Mott scattering of the plane-wave electrons can be found, e.g., in [36, 37, 38, 39]. On the left panel of figure 1, the differential cross section being averaged over μ_i and summed over μ_f is presented. The right panel of figure 1 displays the degree of the longitudinal polarization which is defined by

$$P = \frac{d\sigma_{1/2\ 1/2} - d\sigma_{1/2\ -1/2}}{d\sigma_{1/2\ 1/2} + d\sigma_{1/2\ -1/2}}, \quad (9)$$

where $d\sigma_{\mu_f\mu_i} \equiv \frac{d\sigma_{\mu_f\mu_i}}{d\Omega_f}$ and it is assumed that the incident electron is completely longitudinally polarized ($\mu_i = 1/2$). From this figure, it is seen that both the differential cross section (left panel) and the degree of the longitudinal polarization (right panel) exhibit a strong dependence on the opening angle of the twisted electron. Moreover, one can see that the angular distribution of the emitted electrons has a peak at the angle equal to the opening angle θ_p . This feature of the differential cross section can be exploited for analysis of kinematic properties of the vortex beam. For more details on the Mott scattering of the twisted electrons, we refer to [20, 23].

3.2. Radiative recombination of twisted electrons

We now turn to the consideration of the radiative recombination of the twisted electrons with lead ($Z = 82$) nuclei into the ground $1s$ state of the corresponding H-like ions. In accordance with (7), the differential cross section for this process expresses as

$$\frac{d\sigma_{\chi^m\mu_f\mu_i}^{(tw)}}{d\Omega_k} = \frac{1}{\cos\theta_p} \int \frac{d\varphi_p}{2\pi} \frac{d\sigma_{\chi^m\mu_f\mu_i}^{(pl)}}{d\Omega_k}(\hat{\mathbf{p}}). \quad (10)$$

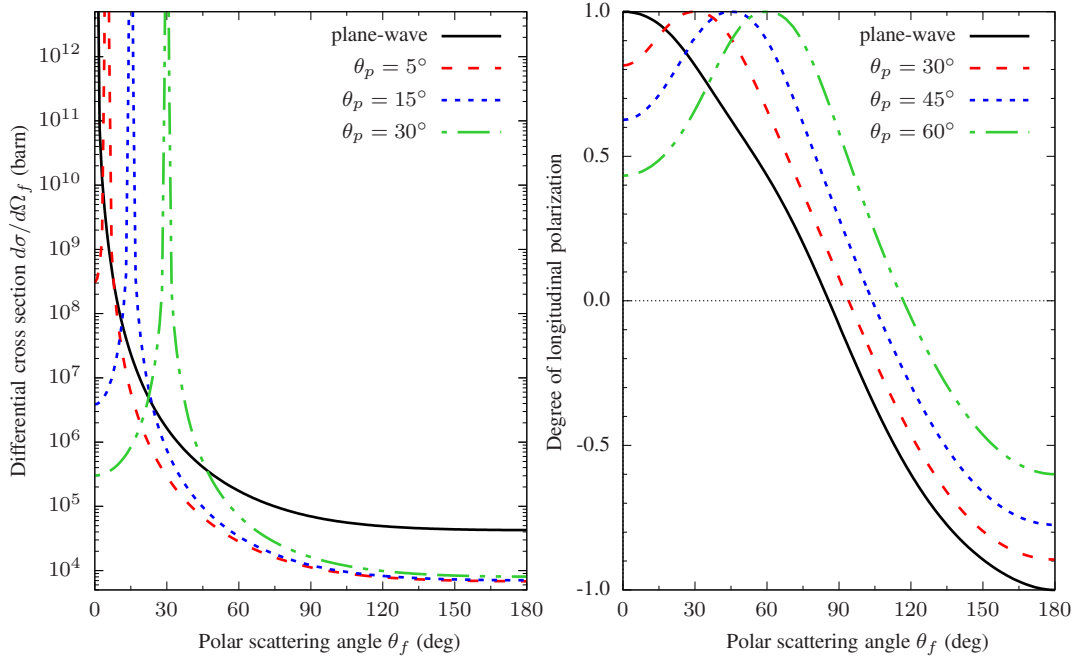


Figure 1. The angular and polarization properties of the electrons emitted in the course of the elastic (Mott) scattering of 100 keV twisted electrons by lead nuclei. On the left panel, the differential cross section (8) averaged over μ_i and summed over μ_f is presented. On the right panel, the degree of the longitudinal polarization (9) is depicted.

Here χ is the angle of the linear polarization of the emitted photon whose solid angle Ω_k is defined by the azimuthal φ_k and polar θ_k angles, and m_f is the TAM projection of the $1s$ electron state. The integral in equation (10) can be readily evaluated with the usage of the well-known expressions from the plane-wave case, which can be found, e.g., in the review [40]. The differential cross section averaged over μ_i and summed over m_f and χ is presented on the left panel of figure 2. From this panel, one can see that the “twistedness” of the incident electron results in qualitative changes of the angular distribution of the emitted photons. Namely, the photons are predominantly emitted in the forward direction, where the plane-wave differential cross-section tends to zero. On the right panel of figure 2 we present the degree of the linear polarization (first Stokes parameter)

$$P_l = P_1 = \frac{d\sigma_{90^\circ} - d\sigma_{0^\circ}}{d\sigma_{90^\circ} + d\sigma_{0^\circ}}, \quad (11)$$

where $d\sigma_\chi \equiv \frac{1}{2} \sum_{m_f \mu_i} \frac{d\sigma_{\chi m_f \mu_i}}{d\Omega_k}$. We note that the second and third Stokes parameters are identically equal to zero. From the right panel of figure 2, it is seen that at large opening angles, the degree of the linear polarization takes negative values. That corresponds to the photons polarized perpendicular to the reaction plane. A similar effect was predicted for the Vavilov-Cherenkov radiation from twisted electrons [41]. More detailed investigations of the radiative recombination of the twisted electrons performed in the first Born approximation and within the fully-relativistic nonperturbative treatment can be found in [16] and [22], respectively.

3.3. Bremsstrahlung from twisted electrons

Let us now briefly discuss the Bremsstrahlung from the twisted electrons scattered by the macroscopic target consisting of bare lead ($Z = 82$) nuclei. With the usage of equation (7), one can obtain the double

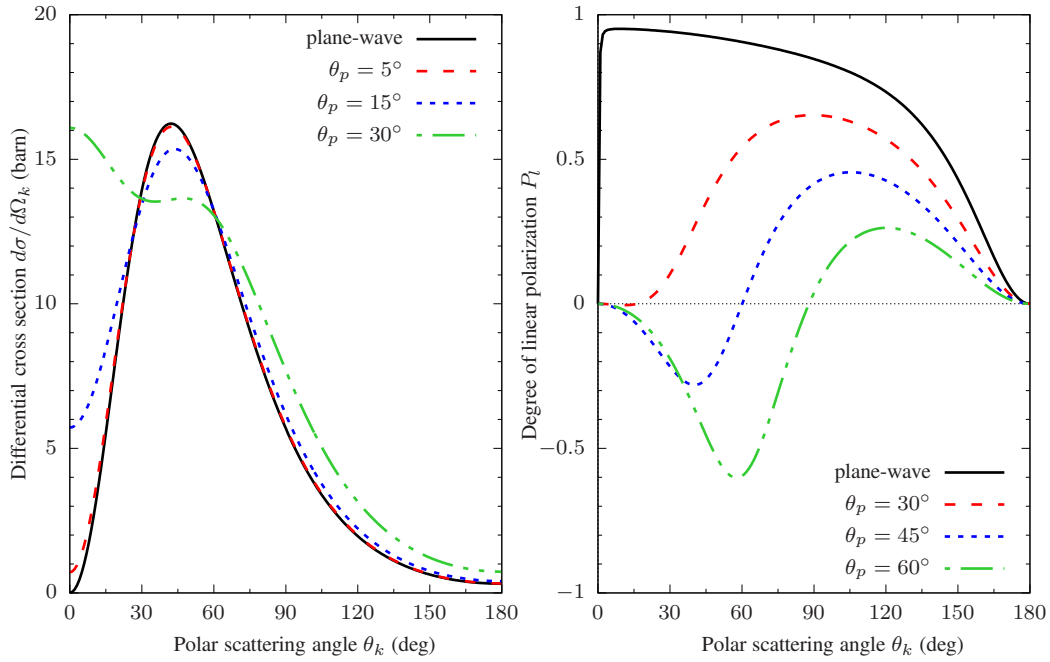


Figure 2. The angular and polarization properties of the photons emitted in the course of the radiative recombination of 100 keV twisted electrons with lead nuclei into the ground $1s$ state of the corresponding H-like ions. On the left panel, the differential cross section (10) averaged over μ_i and summed over m_f and χ is presented. On the right panel, the degree of the linear polarization (11) is depicted.

differential cross section (DDCS) for this process in the following form

$$\frac{d\sigma_{\chi\mu_f\mu_i}^{(tw)}}{d\omega d\Omega_k} = \frac{1}{\cos\theta_p} \int \frac{d\varphi_p}{2\pi} \frac{d\sigma_{\chi\mu_f\mu_i}^{(pl)}}{d\omega d\Omega_k}(\hat{\mathbf{p}}), \quad (12)$$

where ω stands for the energy of the emitted photon. In the present paper, for the evaluation of the plane-wave DDCS, we utilize the theoretical formalism and numerical algorithms developed in [42]. The results of our calculations for the case of 50 keV Bremsstrahlung are presented in figure 3. On the left panel of this figure, the DDCS averaged over μ_i and summed over μ_f and χ is displayed. The right panel of figure 3 demonstrates the degree of the linear polarization (first Stokes parameter), which is defined by a formula similar to (11) with $d\sigma_{\chi} \equiv \frac{1}{2} \sum_{\mu_f\mu_i} \frac{d\sigma_{\chi\mu_f\mu_i}}{d\omega d\Omega_k}$. As in the case of the radiative recombination process, the second and third Stokes parameters are identically equal to zero. From figure 3, it is seen that, the “twistedness” of the incoming electrons leads to qualitative changes of the angular and polarization characteristics. More detailed investigation of the process of the Bremsstrahlung from twisted electrons will be presented in a forthcoming publication.

4. Conclusion

In the present paper, the fundamental atomic processes with twisted electrons were considered. In particular, the elastic (Mott) scattering, the radiative recombination, and the Bremsstrahlung processes were studied within the formalism, which takes into accounts the electron-ion interaction nonperturbatively. This allows one to obtain reliable results even for such heavy systems as lead ($Z = 82$) nuclei. Special attention was paid to the investigation of the influence of the “twistedness” of the incoming electron on the angular and polarization properties of the emitted particles. It was found

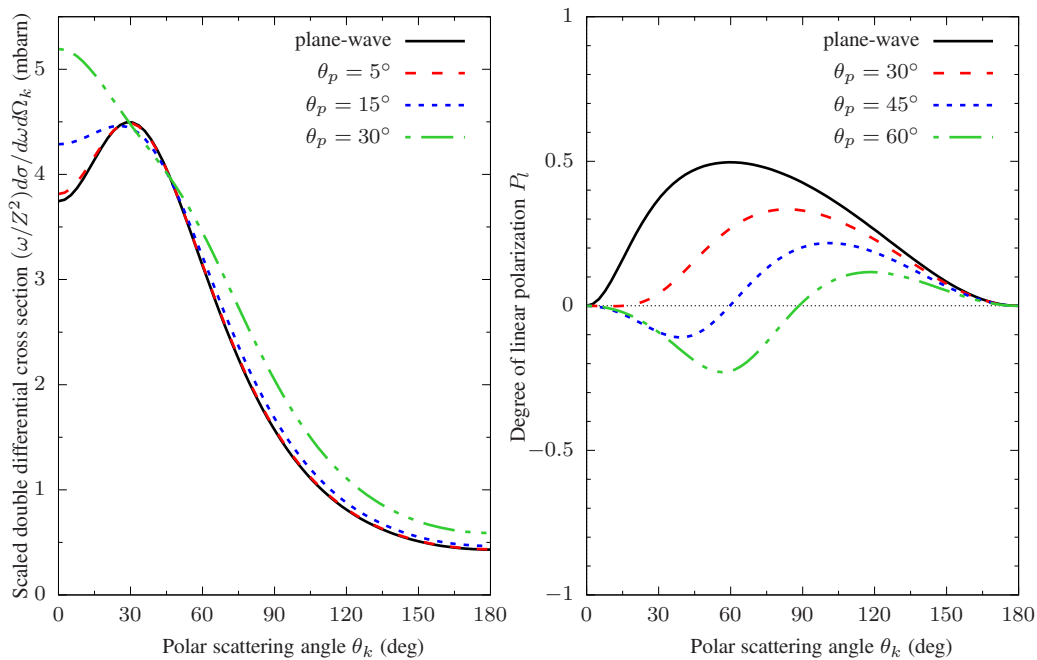


Figure 3. The angular and polarization properties of 50 keV Bremsstrahlung from 100 keV twisted electrons scattered by lead nuclei. On the left panel, the scaled double differential cross section (12) averaged over μ_i and summed over μ_f and χ is presented. On the right panel, the degree of the linear polarization is depicted.

that these properties exhibit a strong dependence on the opening angle of the vortex electron beam in all considered processes.

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