Bremsstrahlung from twisted electrons in the field of heavy nuclei

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We present a fully relativistic calculation of the bremsstrahlung emitted by twisted electrons propagating in the field of bare heavy nuclei. The electron-nucleus interaction is accounted for to all orders in the nuclear binding strength parameter αZ , thus allowing us to investigate the bremsstrahlung in a strong field, where the effects of the "twistedness" are expected to be most pronounced. To explore these effects, we study the angular and polarization properties of the photons emitted in course of the inelastic twisted electrons scattering by the gold target. The influence of the kinematic parameters of the incident electrons on the double-differential cross section and the degree of the linear polarization is also discussed.

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I. INTRODUCTION

The so-called twisted (or vortex) electrons presently attract considerable interest from both experimental and theoretical sides (see [1-3] for a review and relevant references). The interest is partly caused by the fact that the twisted particles can carry a large total angular momentum (TAM) projection $\hbar m$ onto the propagation direction. In particular, twisted electrons with $m \sim 1000$ can be readily produced with current experimental techniques [4]. The magnetic dipole moment of such electrons $m\mu_B$ (μ_B is the Bohr magneton) is by three orders of magnitude larger than one of the plane-wave electrons. As a result, the role of the magnetic interaction in processes involving vortex electron beams is significantly enhanced. This makes twisted electrons a very promising tool for studying magnetic properties of different materials and surfaces [5-8] and for detecting various subtle magnetic effects [9].

All these and other possible applications of twisted electrons are based on properties of fundamental processes of interaction between the twisted beams and atomic targets. Theoretical descriptions of basic atomic processes involving vortex electrons are, therefore, highly demanded. Up to now such descriptions were presented for the radiative recombination [10,11], elastic scattering [12–16], impact excitation [17], and impact ionization [18]. In the present paper, we investigate the bremsstrahlung from twisted electrons by utilizing the fully relativistic description of this process. We follow the formalism developed in Ref. [11] and describe an incoming twisted electron as a coherent superposition of the conventional (plane-wave) electrons propagating in a central potential. As a result, the amplitude of the process is expressed as a coherent sum of the amplitudes of the bremsstrahlung from the plane-wave electrons the evaluation of which can be performed with the usage of well-developed techniques [19–26]. This approach, accounting for the interaction of the incoming and outgoing electrons with the central potential of the target nonperturbatively, allows one to describe the bremsstrahlung from twisted electrons in the field of heavy

atoms. Heavy systems are of particular importance for studies of effects of "twistedness" since one may expect a strong enhancement of these effects due to large spin-orbit interaction.

The paper is organized as follows: In Sec. II A we recall basic relations for the bremsstrahlung from conventional (plane-wave) electrons. The theoretical description of the bremsstrahlung from twisted electrons is presented in Sec. II B. In Secs. III A and III B the numerical results for the double-differential cross section (DDCS) and the Stokes parameters are presented, respectively. Finally, a summary and an outlook are given in Sec. IV.

Relativistic units ($m_e = \hbar = c = 1$) and the Heaviside charge units ($e^2 = 4\pi\alpha$) are utilized in the present paper.

II. BASIC FORMALISM

The description of the bremsstrahlung from twisted electrons can be given in terms of the formulas derived for the plane-wave electrons. We, therefore, start with the compilation of the basic properties of the bremsstrahlung from conventional (plane-wave) electrons. We apply the approach based on the relativistic partial-wave decomposition of the electron's wave function and the multipole expansion of the photon's wave function. This approach is the most appropriate for the description of the bremsstrahlung in the field of heavy systems [19,20,22] where the interaction between the electron and nucleus should be accounted for nonperturbatively.

A. Bremsstrahlung from conventional (plane-wave) electrons

The probability of an emission of a photon with the fourmomentum (ω , **k**) and the polarization λ in the process of the inelastic scattering of an electron with the four-momentum (ε_i , **p**_i) and the helicity μ_i from the bare nucleus is given by [27,28]

$$dW^{(\text{pl})}_{\mu_f,\lambda;\mathbf{p}_i\mu_i} = 2\pi \left| \tau^{(\text{pl})}_{\mu_f,\lambda;\mathbf{p}_i\mu_i} \right|^2 \delta(\varepsilon_i - \varepsilon_f - \omega) d\mathbf{k} d\mathbf{p}_f, \quad (1)$$

where ε_f , \mathbf{p}_f , and μ_f are the energy, the asymptotic momentum, and the helicity of the outgoing electron, respectively.

Here and throughout the average number of the incident particles is set to 1. The amplitude of the bremsstrahlung expresses as

$$\mathbf{r}_{\mu_f,\lambda;\mathbf{p}_i\mu_i}^{(\mathrm{pl})} = \int d\mathbf{r} \Psi_{\mathbf{p}_f\mu_f}^{(-)\dagger}(\mathbf{r}) \hat{R}_{\mathbf{k}\lambda}^{\dagger}(\mathbf{r}) \Psi_{\mathbf{p}_i\mu_i}^{(+)}(\mathbf{r}), \qquad (2)$$

with the photon emission operator given by

$$\hat{R}^{\dagger}_{\mathbf{k}\lambda}(\mathbf{r}) = -\sqrt{\frac{\alpha}{(2\pi)^2\omega}} \boldsymbol{\alpha} \cdot \boldsymbol{\epsilon}^*_{\lambda} e^{-i\mathbf{k}\cdot\mathbf{r}}, \qquad (3)$$

where α stands for the vector of Dirac matrices and the Coulomb gauge defines the polarization vector. The wave functions of the incoming $\Psi_{\mathbf{p}_i\mu_i}^{(+)}$ and outgoing $\Psi_{\mathbf{p}_f\mu_f}^{(-)}$ electrons express as follows [29–31]:

$$\Psi_{\mathbf{p}\mu}^{(\pm)}(\mathbf{r}) = \frac{1}{\sqrt{4\pi p\varepsilon}} \sum_{\kappa m_j} C_{l01/2\mu}^{j\mu} i^l \sqrt{2l+1} e^{\pm i\delta_\kappa} \\ \times D_{m_j\mu}^j(\varphi_{\hat{\mathbf{p}}}, \theta_{\hat{\mathbf{p}}}, 0) \Psi_{\varepsilon \kappa m_j}(\mathbf{r}).$$
(4)

Here $p = |\mathbf{p}|, \kappa = (-1)^{l+j+1/2}(j+1/2)$ is the Dirac quantum number determined by the angular momentum j and the parity $l, C_{j_1m_1 j_2m_2}^{JM}$ is the Clebsch-Gordan coefficient, δ_{κ} is the phase shift induced by the scattering central potential, $D_{MM'}^{J}$ is the Wigner matrix [32,33], the azimuthal $\varphi_{\hat{\mathbf{p}}}$ and polar $\theta_{\hat{\mathbf{p}}}$ angles define the direction of the unit vector $\hat{\mathbf{p}}$, and $\Psi_{\varepsilon\kappa m_j}$ is the partial-wave Dirac solution (so-called Coulomb-distorted waves), the explicit form of which can be found, e.g., in Refs. [27,28].

Substituting Eq. (4) into Eq. (2) and utilizing the well-known multipole expansion for the photon emission operator (3), we obtain the final expression in the form of the triple expansion over the electron partial waves and photon multipoles. The partial amplitudes, i.e., terms of this sum, are evaluated by separating the angular integration and performing it analytically. The remaining integral over the radial variable has to be calculated numerically (see, e.g., Ref. [22]). Summing over the partial waves and multipoles up to desired accuracy, we determine the bremsstrahlung amplitude which defines the probability (1) and, consequently, all the properties of the process studied.

B. Bremsstrahlung from twisted electrons

The theoretical description of the free twisted electrons is well represented in the literature (see [1–3] for a review and relevant references). Here we only briefly sketch the important properties of these electrons, which are taken in the form of a Bessel wave in the present paper. Twisted electrons possess the well-defined energy ε , helicity μ , and the total angular *m* and linear p_z momenta projections onto the same direction. The *z* axis is fixed along this direction. In the momentum space, these states represent a cone with the opening angle $\theta_p = \arctan(\varkappa/p_z)$ where $\varkappa = \sqrt{\varepsilon^2 - 1 - p_z^2}$ stands for the well-defined transversal momentum. The Bessel vortex electron can be described by the following wave function [13]:

$$\psi_{\varkappa m p_{z}\mu}(\mathbf{r}) = \int d\mathbf{p} \frac{e^{im\varphi_{p}}}{2\pi p_{\perp}} \delta(p_{\parallel} - p_{z}) \delta(p_{\perp} - \varkappa) i^{\mu - m} \psi_{\mathbf{p}\mu}(\mathbf{r}),$$
(5)



FIG. 1. The geometry of the bremsstrahlung from twisted electrons in the field of a single bare nucleus shifted from the z axis by the impact parameter **b**.

where p_{\parallel} (p_{\perp}) is the longitudinal (perpendicular) component of the momentum **p** and the wave function of the plane-wave electron is given by

$$\psi_{\mathbf{p}\mu}(\mathbf{r}) = \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{(2\pi)^3}} U_{\mathbf{p}\mu},\tag{6}$$

with $U_{\mathbf{p}\mu}$ standing for the Dirac bispinor [28]:

$$U_{\mathbf{p}\mu} = \frac{1}{\sqrt{2\varepsilon}} \left(\frac{\sqrt{\varepsilon + 1} \chi_{1/2\mu}(\hat{\mathbf{p}})}{\sqrt{\varepsilon - 1}(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) \chi_{1/2\mu}(\hat{\mathbf{p}})} \right).$$
(7)

Here $\boldsymbol{\sigma}$ is the vector of Pauli matrices, and $\chi_{1/2\mu}(\hat{\mathbf{p}})$ is the eigenfunction of the helicity operator $(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})/2$ with the eigenvalue μ . Utilizing Eq. (5), one can unfold other distinguishing features of the twisted electrons, namely, the inhomogeneity of the probability distribution and the flux density with respect to the space variable. As an example, the flux density is given by

$$j_{z}^{(\text{tw})} = \psi_{\varkappa m p_{z} \mu}^{\dagger}(\mathbf{r}) \alpha_{z} \psi_{\varkappa m p_{z} \mu}(\mathbf{r})$$
$$= \frac{p}{\varepsilon (2\pi)^{3}} \sum_{\sigma} 4\mu \sigma \left[d_{\sigma \mu}^{1/2}(\theta_{p}) J_{m-\sigma}(\varkappa r_{\perp}) \right]^{2}, \quad (8)$$

where $d_{MM'}^J(\theta)$ is the small Wigner matrix [32,33], J_{ν} is the Bessel function of the first kind [34,35], and $r_{\perp} = |\mathbf{r}_{\perp}|$ with \mathbf{r}_{\perp} being the perpendicular component of \mathbf{r} . These features result in the dependence of the scattering process on the relative position of the target and the vortex beam.

We start with the consideration of the bremsstrahlung from twisted electrons in the field of a single bare nucleus, which is shifted from the *z* axis by the impact parameter $\mathbf{b} = (b_x, b_y, 0)$ as shown in Fig. 1. Here and below we assume that both the emitted photon and the outgoing electron are asymptotically described by the plane waves. This corresponds to the assumption that detectors used in the actual experiments do not register "twistedness" of the particles, which is the case for the present-day experimental setups. The probability of the process depicted in Fig. 1 is given by

$$dW^{(\text{tw})}_{\mu_{f},\lambda;\varkappa mp_{z}\mu_{i}}(\mathbf{b})$$

= $2\pi \left| \tau^{(\text{tw})}_{\mu_{f},\lambda;\varkappa mp_{z}\mu_{i}}(\mathbf{b}) \right|^{2} \delta(\varepsilon_{i} - \varepsilon_{f} - \omega) d\mathbf{k} d\mathbf{p}_{f}, \quad (9)$



FIG. 2. Geometry of the bremsstrahlung process from twisted electrons scattered by a macroscopic target.

with the scattering amplitude expressing as

$$\tau_{\mu_{f},\lambda;\varkappa mp_{z}\mu_{i}}^{(\mathrm{tw})}(\mathbf{b}) = \int d\mathbf{r} \Psi_{\mathbf{p}_{f}\mu_{f}}^{(-)\dagger}(\mathbf{r}-\mathbf{b}) \hat{R}_{\mathbf{k}\lambda}^{\dagger}(\mathbf{r}-\mathbf{b}) \Psi_{\varkappa mp_{z}\mu_{i}}^{(+)}(\mathbf{r})$$
$$= \int d\mathbf{r} \Psi_{\mathbf{p}_{f}\mu_{f}}^{(-)\dagger}(\mathbf{r}) \hat{R}_{\mathbf{k}\lambda}^{\dagger}(\mathbf{r}) \Psi_{\varkappa mp_{z}\mu_{i}}^{(+)}(\mathbf{r}+\mathbf{b}). (10)$$

The explicit form of the wave function of the asymptotically twisted electron propagating in the central field can be found in Ref. [11]:

$$\Psi_{\varkappa m p_{z} \mu_{i}}^{(+)}(\mathbf{r}+\mathbf{b}) = \int d\mathbf{p} \frac{e^{im\varphi_{p}}}{2\pi p_{\perp}} \delta(p_{\perp}-\varkappa) \delta(p_{\parallel}-p_{z}) i^{\mu_{i}-m} \times \Psi_{\mathbf{p}\mu_{i}}^{(+)}(\mathbf{r}) e^{i\mathbf{p}\cdot\mathbf{b}}.$$
(11)

Substituting Eq. (11) into Eq. (10) one can express the amplitude of the bremsstrahlung from the twisted electron through the one appearing in the plane-wave case (2):

$$\tau_{\mu_{f},\lambda;\varkappa mp_{z}\mu_{i}}^{(\mathrm{tw})}(\mathbf{b}) = \int d\mathbf{p} \frac{e^{im\varphi_{p}}}{2\pi p_{\perp}} \delta(p_{\perp} - \varkappa) \\ \times \delta(p_{\parallel} - p_{z}) i^{\mu_{i} - m} e^{i\mathbf{p}\cdot\mathbf{b}} \tau_{\mathbf{p}_{f}\mu_{f},\mathbf{k}\lambda;\mathbf{p}\mu_{i}}^{(\mathrm{pl})}.$$
(12)

The scattering amplitude (12) defines uniquely the probability of the process under consideration, from which all measurable quantities can be determined.

Up to now we have considered the bremsstrahlung from twisted electrons in a field of a single ionic or atomic target. The experimental investigation of such a process is a challenging task. We now consider a more realistic scenario, namely, the bremsstrahlung from the twisted electrons scattered by the infinitely extended (macroscopic) target. We describe this target as an incoherent superposition of ions (or atoms) being randomly and homogeneously distributed. The fully differential cross section of this scenario being schematically depicted in Fig. 2 is given by [13]

$$\frac{d\sigma_{\mu_f,\lambda; \approx p_z \mu_i}^{(\text{tw})}}{d\omega d\Omega_k d\Omega_f} = \frac{1}{J_z^{(\text{tw})}} \int \frac{d\mathbf{b}}{\pi R^2} \frac{dW_{\mu_f,\lambda; \approx m p_z \mu_i}^{(\text{tw})}(\mathbf{b})}{d\omega d\Omega_k d\Omega_f}$$
$$= \frac{1}{\cos \theta_p} \int \frac{d\varphi_p}{2\pi} \frac{d\sigma_{\mu_f,\lambda; \mathbf{p} \mu_i}^{(\text{pl})}}{d\omega d\Omega_k d\Omega_f}, \quad (13)$$

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where $J_z^{(tw)}$ is the averaged flux the explicit form of which will be specified below, πR^2 is the cross-section area with *R* being the radius of the cylindrical box, and

$$\frac{d\sigma_{\mu_f,\lambda;\mathbf{p}_i\mu_i}^{(\mathrm{pl})}}{d\omega d\Omega_k d\Omega_f} = \frac{(2\pi)^3}{v_i} \frac{dW_{\mu_f,\lambda;\mathbf{p}_i\mu_i}^{(\mathrm{pl})}}{d\omega d\Omega_k d\Omega_f}$$
$$= (2\pi)^4 \omega^2 \frac{P_f \varepsilon_f}{v_i} |\tau_{\mu_f,\lambda;\mathbf{p}_i\mu_i}^{(\mathrm{pl})}|^2 \qquad (14)$$

is the fully differential cross section of the bremsstrahlung from plane-wave electrons with the velocity v_i . The averaged flux of the incoming twisted electrons is given by

$$J_z^{(\text{tw})} = \int \frac{d\mathbf{r}_\perp}{\pi R^2} j_z^{(\text{tw})} = \frac{v_i}{(2\pi)^3} \frac{2}{\pi R \varkappa} \cos \theta_p.$$
(15)

From Eq. (13) it is seen that in the case of the scattering of the twisted electron by the macroscopic target the fully differential cross section does not depend on the projection m of TAM.

In the present investigation, we restrict ourselves to the consideration of the scenario in which the incoming twisted electron is spin unpolarized and only the emitted photon is detected. This process is described by the DDCS

$$d\sigma_{\lambda} \equiv \frac{d\sigma_{\lambda;\varkappa p_{z}}^{(\text{tw})}}{d\omega d\Omega_{k}} = \frac{1}{2} \sum_{\mu_{i}\mu_{f}} \int d\Omega_{f} \frac{d\sigma_{\mu_{f},\lambda;\varkappa p_{z}\mu_{i}}}{d\omega d\Omega_{k} d\Omega_{f}}$$
$$= \frac{1}{\cos\theta_{p}} \int \frac{d\varphi_{p}}{2\pi} \frac{d\sigma_{\lambda;\mathbf{p}}^{(\text{pl})}}{d\omega d\Omega_{k}}, \quad (16)$$

where

$$\frac{d\sigma_{\lambda;\mathbf{p}_i}^{(\mathrm{pl})}}{d\omega d\Omega_k} = \frac{1}{2} \sum_{\mu_i \mu_f} \int d\Omega_f \frac{d\sigma_{\mu_f,\lambda;\mathbf{p}_i \mu_i}^{(\mathrm{pl})}}{d\omega d\Omega_k d\Omega_f}$$
(17)

is the DDCS for the bremsstrahlung from plane-wave electrons.

III. RESULTS AND DISCUSSIONS

As already has been mentioned the effects of the "twistedness" are expected to be most pronounced for heavy systems. We consider, therefore, the bremsstrahlung from twisted electrons scattered by an ionic (or atomic) gold target. The energies of the incident electrons are chosen to be 100 and 500 keV. At such energies, the bremsstrahlung from electrons comes mostly from the nuclei [22]. In what follows, we study the scattering of twisted electrons by an infinite macroscopic target consisting of bare gold nuclei, assuming the scattering on the electronic shells surrounding the nuclei to be negligible. This choice of our model allows us to explicitly demonstrate the effects induced by the "twistedness" of the incident electron.

A. Double-differential cross section

We start from the analysis of the DDCS for the bremsstrahlung from 100- and 500-keV twisted electrons scattered by the macroscopic target consisting of bare gold



FIG. 3. The scaled DDCS $d\sigma \equiv (\omega/Z^2) \sum_{\lambda} d\sigma_{\lambda}$ for the bremsstrahlung from the twisted electrons with the opening (conical) angle θ_p and the energy $\varepsilon_i = 100$ keV (first row) and 500 keV (second row) as a function of the photon emission angle θ_k . The left, middle, and right panels correspond to the energies of the outgoing electron $\varepsilon_f = 0.01\varepsilon_i$, $0.1\varepsilon_i$, and $0.5\varepsilon_i$, respectively.

(Z = 79) nuclei. Figure 3 presents the DDCS (16) summed over λ for three different energies of the outgoing electron $\varepsilon_f = 0.01\varepsilon_i$, $0.1\varepsilon_i$, and $0.5\varepsilon_i$. From this figure, it is seen that the growth of the opening angle θ_p leads to the strong qualitative changes in the angular distribution of the bremsstrahlung. These changes, however, manifest differently for different energies of the incident electron. Indeed, for $\varepsilon_i =$ 100 keV (first row in Fig. 3) the probability of the forward bremsstrahlung increases with the growth of the opening angle and at $\theta_p \gtrsim 30^\circ$ the DDCS turns into a monotonically decreasing function with a maximum at $\theta_k = 0^\circ$. In contrast to this, for $\varepsilon_i = 500$ keV (second row in Fig. 3) the increase of the opening angle leads to the drop of the probability of the forward bremsstrahlung. The most significant change of the DDCS for this incident electron energy happens at $\varepsilon_f =$ 0.5 and $\theta_p = 45^\circ$. For these parameters, the formation of a maximum at the photon emission angles θ_k from 30° to 60° is predicted.

B. Stokes parameters

We now turn to the investigation of the "twistedness"induced effects on the polarization properties of the bremsstrahlung. For this purpose, we evaluate the Stokes parameters which are defined as

$$P_{1} = \frac{d\sigma_{0^{\circ}} - d\sigma_{90^{\circ}}}{d\sigma_{0^{\circ}} + d\sigma_{90^{\circ}}}, \quad P_{2} = \frac{d\sigma_{45^{\circ}} - d\sigma_{135^{\circ}}}{d\sigma_{45^{\circ}} + d\sigma_{135^{\circ}}},$$
$$P_{3} = \frac{d\sigma_{+1} - d\sigma_{-1}}{d\sigma_{+1} + d\sigma_{-1}}.$$
(18)

Here $d\sigma_{\chi}$ is the DDCS from Eq. (16) for the emission of a photon with linear polarization ϵ_{χ} , characterized by the angle χ , while $d\sigma_{+1}$ and $d\sigma_{-1}$ are the cross sections for the emission of a right circularly and left circularly polarized photon, respectively [22,36].

Figure 4 presents the degree of the linear polarization (the first Stokes parameter P_1) for the bremsstrahlung from twisted electrons with energy $\varepsilon_i = 100$ and 500 keV, scattered by a macroscopic target consisting of bare gold (Z = 79) nuclei. We note that for the process under investigation P_2 and P_3 are identically equal to zero, that is the consequence of the fact that the electron beam is unpolarized [20]. From Fig. 4 it is seen that, like in the case of the DDCS (see Fig. 3), the degree of the linear polarization exhibits a strong dependence on the kinematic parameters of the incident twisted electron. As an example, for the 100-keV incident electron energy (first row in Fig. 4) and $\theta_p = 45^\circ$, the first Stokes parameter P_1 takes



FIG. 4. The degree of the linear polarization (the first Stokes parameter P_1) for the bremsstrahlung from the twisted electrons with the opening (conical) angle θ_p and the energy $\varepsilon_i = 100$ keV (first row) and 500 keV (second row) as a function of the photon emission angle θ_k . The left, middle, and right panels correspond to the energies of the outgoing electron $\varepsilon_f = 0.01\varepsilon_i$, $0.1\varepsilon_i$, and $0.5\varepsilon_i$, respectively.

negative values. This corresponds to the bremsstrahlung which is linearly polarized perpendicular to the scattering plane. A similar effect was predicted for the Vavilov-Cherenkov radiation by twisted electrons [37] and for the radiative recombination of twisted electrons [11]. For $\varepsilon_i = 500 \text{ keV}$ (second row in Fig. 4) we observe a more pronounced dependence on the opening (conical) angle θ_p . Already at θ_p from 15° to 30°, the degree of the linear polarization undergoes qualitative changes when compared to the planewave case. Such a strong dependence of the first Stokes parameter P_1 on the opening angle allows one to consider the bremsstrahlung process as a possible tool for the diagnostics of the twisted electron beams.

IV. CONCLUSION

In this paper we have developed a fully relativistic description of the bremsstrahlung by twisted electrons in the field of heavy nuclei. Our approach accounts for the interaction of the incoming vortex and outgoing plane-wave electrons with the Coulomb field of the target to all orders in the nuclear binding strength parameter αZ .

The developed approach has been applied for the investigation of the angular and polarization properties of the bremsstrahlung from twisted electrons scattered by the macroscopic target consisting of bare gold nuclei. In particular, the double-differential cross section and the degree of linear polarization P_1 of the bremsstrahlung as functions of the photon emission angle were evaluated for different energies of the outgoing electron. It was found that both the DDCS and P_1 do depend strongly on the kinematic properties of the twisted electron, namely, the opening angle θ_p and the energy ε_i . Additionally, the dependence on θ_p is qualitatively different for different incident electron energies. As an example, for $\varepsilon_i = 100$ keV the forward bremsstrahlung increases with the growth of θ_p , while for $\varepsilon_i = 500$ keV it decreases. It was also found that P_1 exhibits a stronger dependence on θ_p for 500-keV twisted electrons when compared to the 100-keV ones.

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