Polarization studies on Rayleigh scattering of hard x rays by closed-shell atoms

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We present a theoretical study on the elastic Rayleigh scattering of x-ray photons by closed-shell atoms. Special attention is paid to the transfer of linear polarization from the incident to the outgoing photons. To study this process, we apply the density-matrix formalism combined with the relativistic perturbation theory. This formalism enables us to find general relations between the Stokes parameters of the incident and scattered photons. By using these expressions, we revisit the recent proposal to use Rayleigh scattering for the analysis of the polarization purity of synchrotron radiation. We show that this analysis can be performed without any need for the theoretically calculated scattering amplitudes, if the linear polarization of the scattered light is measured simultaneously at the azimuthal angles 0° and 45° with respect to the plane of the synchrotron. To illustrate our approach, we present detailed calculations for scattering of 145 keV photons by lead atoms.

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I. INTRODUCTION

Owing to the recent advancements in developing the third generation coherent light sources, new possibilities have arisen to study elastic scattering of x rays by atomic targets to which three basic processes contribute: Nuclear Thomson, Rayleigh, and Delbrück scattering [1]. In the hard-x-ray range from a few keV to 1 MeV, Rayleigh scattering of photons by bound atomic electrons is the dominant process. In the past, mainly the total as well as the angular differential Rayleigh scattering cross section have been studied [1–5]. These cross sections are of general interest but are also needed to determine the Delbrück scattering cross sections [6,7]. During the recent years, moreover, special attention was paid to the polarization of the elastically scattered photons [8,9]. These polarization studies have not only allowed us to reveal more information about the electron-photon interaction in the high-energy regime, but can also be used for the diagnostics of the incident photon beams [10–12]. In particular, a very strong correlation of the polarization of incoming and outgoing photons has been found for Rayleigh scattering. This polarization correlation made it possible to propose Rayleigh scattering as a tool for precise polarization measurements. The feasibility of this Rayleigh polarimetry scheme has been recently demonstrated in the experiment performed at the PETRA III synchrotron facility at DESY [11,13]. In this experiment, where 175 keV photons were scattered by a gold target, the polarization-resolved measurements of the elastically scattered photons have allowed us to obtain the polarization purity of synchrotron radiation [11,12]. It was found that the linear polarization of the synchrotron radiation emitted within the plane of the ring is about 98%, which deviates from the naive expectation of 100% [11].

The Rayleigh polarimetry method mentioned above cannot be performed without the theoretical calculations of the elastic-scattering amplitudes [1,10,11]. These second-order calculations are a complicated task, especially for many-electron target atoms, usually used in experiments. Therefore, theoretical input can introduce additional uncertainties in the polarization purity analysis. To overcome the need of theoretical data, we develop a more advanced polarimetry scheme based on Rayleigh scattering. A first step towards this development has been made in Ref. [10], where we proposed simultaneous measurements of the linear polarization and the angular distribution of the elastically scattered photons. However, precise measurements of scattering cross sections under various observation angles tend to be laborious for experimentalists because several possible sources of systematic uncertainties, such as detector efficiency, solid angle coverage, and incident photon flux, need to be under rigorous control.

In this work, we propose an alternative approach, which is based on the concurrent measurement of the linear polarization of photons scattered *within* the synchrotron plane and under the angle of 45° with respect to the synchrotron. The advantage of this scheme is that it is based on the well-established Compton polarimetry technique and can be easily realized at the present facilities like PETRA III at DESY.

To analyze the polarization transfer in Rayleigh scattering, we discuss in Sec. II the geometry of this elastic process. Later in Sec. III A we continue with the theoretical discussion of the Rayleigh scattering amplitudes. The application of this second-order matrix element for the evaluation of the density matrix of the scattered light is discussed in Sec. III B. The advantage of the density matrix is that it enables us to show how the Stokes parameters of incident and outgoing photons

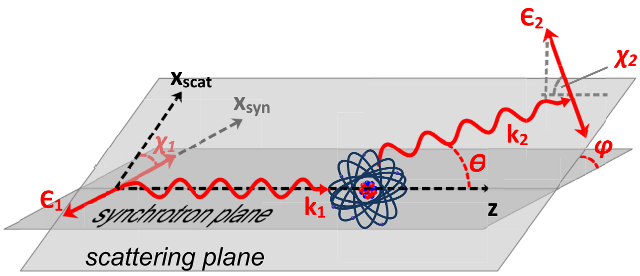

FIG. 1. The geometry of Rayleigh scattering. The propagation direction of the incident light is chosen as the z axis. Together with the incident linear polarization vector $\boldsymbol{\epsilon}_1$, the z axis defines the synchrotron plane. For the theoretical description, the plane, spanned by the propagation directions of incident and outgoing photons, is important. This plane is usually referred to as the scattering plane.

can be related to each other. In Sec. IV, we present the details of our numerical calculations. Furthermore, in Sec. V, we discuss the Stokes parameters for a typical synchrotron setup. We performed detailed calculations for 145 keV photons scattered off lead atoms. In particular, we suggest, based on these results, to make two polarization-sensitive measurements at two different azimuthal angles, 0° and 45° with respect to the plane of the synchrotron to determine the incident polarization. For the least uncertainty, the scattered photons should be detected at the polar angle 70° or 105°. The summary of these results is presented in Sec. VI.

II. GEOMETRY

Before we present the theory to describe Rayleigh scattering, we first introduce the geometry of this process. We consider the typical setup of an elastic photon-atom scattering experiment as performed at synchrotron facilities such as PETRA III at DESY. In this setup, the incoming x rays are almost completely linearly polarized within the plane of the synchrotron ring. We will denote this plane as the synchrotron plane, in which the x and z axes are chosen along the polarization and wave vectors $\boldsymbol{\epsilon}_1$ and $\boldsymbol{k}_1$ of the incident radiation. In this coordinate system, the direction of the scattered photons is characterized by the angles θ and φ. While the polar angle θ is defined with respect to the z axis, the angle φ is the azimuthal angle between the wave vector of the scattered photon $\boldsymbol{k}_2$ and the xz plane.

The synchrotron plane describes the setup as seen from an experimental viewpoint. For the theoretical description of the scattering process, however, it is more convenient to use another coordinate system. In this case the xz plane is spanned by the wave vectors of the incoming and outgoing photons, $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$. This plane will be denoted as the scattering plane. The tilt angle between both planes is the azimuthal angle φ, as seen from Fig. 1. The azimuthal angle between the polarization vectors of the initial and scattered photon, $\boldsymbol{\epsilon}_1$ and $\boldsymbol{\epsilon}_2$, and the scattering plane are called χ_1 and χ_2, respectively. We note that, for the particular case shown here, $\chi_1 = \varphi$.

III. THEORETICAL BACKGROUND

After discussing the geometry of the Rayleigh scattering process, we are ready to present its basic theory. We start our discussion from the scattering amplitude, which is the main quantity for the evaluation of the polarization properties of the scattered photons, and we show how this many-body amplitude can be evaluated within the independent-particle approximation (IPA). Later, this amplitude will be used to calculate the Stokes parameters of the scattered photons for an arbitrary polarization of the incident light.

A. Scattering amplitudes

1. Scattering amplitudes in helicity representation

In this section, we calculate the scattering amplitude of Rayleigh scattering. Using second-order perturbation theory, we obtain

$$M_{fi}(\boldsymbol{k}_1, \lambda_1, \boldsymbol{k}_2, \lambda_2) = \sum_{\alpha_\nu J_\nu M_\nu} \left\{ \frac{\langle \alpha_f J_f M_f | \hat{R}^\dagger_{\lambda_2}(\boldsymbol{k}_2) | \alpha_\nu J_\nu M_\nu \rangle \langle \alpha_\nu J_\nu M_\nu | \hat{R}_{\lambda_1}(\boldsymbol{k}_1) | \alpha_i J_i M_i \rangle}{E_i + \omega_1 - E_\nu} + \frac{\langle \alpha_f J_f M_f | \hat{R}_{\lambda_1}(\boldsymbol{k}_1) | \alpha_\nu J_\nu M_\nu \rangle \langle \alpha_\nu J_\nu M_\nu | \hat{R}^\dagger_{\lambda_2}(\boldsymbol{k}_2) | \alpha_i J_i M_i \rangle}{E_i - \omega_2 - E_\nu} \right\}, \tag{1}$$

where $\boldsymbol{k}_{1,2}$ and $\boldsymbol{\epsilon}_{1,2}$ are the wave- and polarization-vectors of the incident and outgoing light [1]. The initial, intermediate, and final states $|\alpha_i J_i M_i\rangle$, $|\alpha_\nu J_\nu M_\nu\rangle$, and $|\alpha_f J_f M_f\rangle$ are characterized by their energy E, the total angular momentum J, and its projection M. Moreover, α is used as a shorthand notation for all other quantum numbers needed for the unique specification of the atomic state. In the denominator, ω_1 and ω_2 are the energies of the incident and outgoing photons, respectively.

The absorption and emission of photons with well-defined helicity by an atom in Eq. (1) are described by the operators $\hat{R}_\lambda$ and $\hat{R}^\dagger_\lambda$. These operators can be written as a sum of their one-electron counterparts:

$$\hat{R}_\lambda(\boldsymbol{k}) = \sum_n \boldsymbol{\alpha}_n \boldsymbol{\epsilon}_\lambda e^{i\boldsymbol{k}\boldsymbol{r}_n}, \tag{2}$$

where $\boldsymbol{\alpha}_n$ and $\boldsymbol{r}_n$ are the vector of Dirac matrices and coordinate vectors of the nth electron, respectively. The polarization vector $\boldsymbol{\epsilon}_\lambda$ describes the right- ($\lambda = -1$) or the left-handed ($\lambda = +1$) circular polarization, with $\lambda = \pm 1$ being the helicity of the photon [14].

In general, the Rayleigh amplitudes for scattering off closed-shell systems ($J_i = J_f = 0$) possess an important symmetry property:

$$M_{fi}(\boldsymbol{k}_1, \lambda_1, \boldsymbol{k}_2, \lambda_2) = M_{fi}(\boldsymbol{k}_1, -\lambda_1, \boldsymbol{k}_2, -\lambda_2). \quad (3)$$

This expression implies that, for given $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$, only two independent scattering amplitudes are needed to describe the Rayleigh process. In the next section, we see how these amplitudes can be obtained in the linear polarization basis.

2. Scattering amplitudes for linearly polarized photons

The Rayleigh scattering amplitudes for circularly polarized incoming and outcoming photons are represented by Eqs. (1) and (2). In modern synchrotron experiments, however, the incident light is almost fully linearly polarized and the detectors for the scattered photons are able to measure the linear polarization. To describe these experiments, it is therefore convenient to rewrite M_{fi} in the linear polarization basis. To achieve this, we use the standard relation between circular and linear polarization vectors,

$$\boldsymbol{\epsilon}_l = \frac{1}{\sqrt{2}} \sum_\lambda e^{-i\lambda\chi} \boldsymbol{\epsilon}_\lambda, \quad (4)$$

where we follow the convention introduced by Rose [14]. In this expression, moreover, χ is the azimuthal angle between the linear polarization vector $\boldsymbol{\epsilon}_l$ and the scattering plane, see Fig. 1. By inserting the expansion (4) into Eq. (1) and performing some simple algebra, we obtain

$$M_{fi}(\boldsymbol{k}_1, \chi_1, \boldsymbol{k}_2, \chi_2) = \frac{1}{2} \sum_{\lambda_1,\lambda_2} e^{-i(\lambda_1\chi_1 - \lambda_2\chi_2)} \times M_{fi}(\boldsymbol{k}_1, \lambda_1, \boldsymbol{k}_2, \lambda_2). \quad (5)$$

While Eq. (5) can be applied to describe the scattering of photons with arbitrary linear polarization, it is convenient to consider four linearly independent amplitudes: $M_{fi}(\boldsymbol{k}_1, \chi_1 = 0^\circ, \boldsymbol{k}_2, \chi_2 = 0^\circ)$, $M_{fi}(\boldsymbol{k}_1, \chi_1 = 90^\circ, \boldsymbol{k}_2, \chi_2 = 90^\circ)$, $M_{fi}(\boldsymbol{k}_1, \chi_1 = 0^\circ, \boldsymbol{k}_2, \chi_2 = 90^\circ)$, and $M_{fi}(\boldsymbol{k}_1, \chi_1 = 90^\circ, \boldsymbol{k}_2, \chi_2 = 0^\circ)$. Owing to the symmetry property of the matrix elements (3), only the first two of these amplitudes are nonzero. In the literature, these two amplitudes are often denoted $A_\parallel$ and $A_\perp$ for the cases where the incoming and outgoing photons are polarized either parallel or perpendicular to the scattering plane (see, for example, Refs. [1,3,10]). We now introduce the ratio of the two independent amplitudes:

$$S(\omega, \theta) \equiv S = \frac{A_\parallel}{A_\perp}. \quad (6)$$

This ratio depends on the photon energy $\omega = \omega_1 = \omega_2$, the scattering angle θ, as well as on the electronic structure of the target atom, and it is of particular importance since it defines many polarization properties of the Rayleigh scattering, as will be shown below.

B. Density-matrix formalism

Having discussed the evaluation of the scattering amplitude both in the circular and in linear polarization basis, we proceed to the analysis of the Stokes parameters of Rayleigh scattered light. Most naturally, this analysis can be performed within the framework of density-matrix theory. In this theory, the initial and final states of the system are described by means of the so-called statistical operators $\hat{\rho}_i$ and $\hat{\rho}_f$, which are related to each other as

$$\hat{\rho}_f = \hat{T} \hat{\rho}_i \hat{T}^\dagger. \quad (7)$$

The transition operator $\hat{T}$ describes the interaction between photons and bound electrons during the scattering [15,16].

For practical reasons, it is convenient to rewrite Eq. (7) in matrix form. To achieve this, we have to agree about the representation of the matrix of operators $\hat{\rho}$, which is known as the density matrix. It is very useful to express this matrix in the photon helicity representation. In this representation, the density matrix of a photon scattered off a closed-shell atom can be written as

$$\langle \boldsymbol{k}_2\lambda_2|\hat{\rho}_f|\boldsymbol{k}_2\lambda_2'\rangle = \sum_{\lambda_1,\lambda_1'} \langle \boldsymbol{k}_1\lambda_1|\hat{\rho}_i|\boldsymbol{k}_1\lambda_1'\rangle \langle \alpha_i J_i M_i, \boldsymbol{k}_1\lambda_1'|\hat{T}^+|\alpha_f J_f M_f, \boldsymbol{k}_2\lambda_2'\rangle \langle \alpha_f J_f M_f, \boldsymbol{k}_2\lambda_2|\hat{T}|\alpha_i J_i M_i, \boldsymbol{k}_1\lambda_1\rangle$$
$$= \mathcal{C} \sum_{\lambda_1,\lambda_1'} \langle \boldsymbol{k}_1\lambda_1|\hat{\rho}_i|\boldsymbol{k}_1\lambda_1'\rangle M^*_{fi}(\boldsymbol{k}_1, \lambda_1', \boldsymbol{k}_2, \lambda_2')\, M_{fi}(\boldsymbol{k}_1, \lambda_1, \boldsymbol{k}_2, \lambda_2), \quad (8)$$

where we use the fact that the matrix elements of the transition operator $\hat{T}$ are proportional to the second-order scattering amplitude (1) and $J_i = J_f = M_i = M_f = 0$.

In the helicity representation (8), the density matrix of incident and outgoing photons can be parametrized in terms of the so-called Stokes parameters as follows:

$$\langle \boldsymbol{k}\lambda|\hat{\rho}|\boldsymbol{k}\lambda'\rangle = \begin{pmatrix} 1 + P_3 & P_1 - iP_2 \\ P_1 + iP_2 & 1 - P_3 \end{pmatrix}. \quad (9)$$

As usual in atomic physics, the Stokes parameters P_1 and P_2 are expressed in terms of intensities I of light, linearly polarized under different angles with respect to the scattering plane. For instance, the parameter $P_1 = [I(0^\circ) - I(90^\circ)]/[I(0^\circ) + I(90^\circ)]$ characterizes the light, which is linearly polarized within or perpendicular to the scattering plane. The Stokes parameter P_2 is obtained from the analogous expression for tilt angles of 45° and 135°. Finally, the degree of circular polarization is characterized by the parameter $P_3 = [I(\lambda = +1) - I(\lambda = -1)]/[I(\lambda = +1) + I(\lambda = -1)]$ [14]. As already mentioned above, the present work focuses especially on the linear polarization of incoming and outgoing photons. The polarization of a photon can be illustrated by the polarization ellipse. The semimajor axis of this ellipse is related to the Stokes parameters via $P_l = (P_1^2 + P_2^2)^{1/2}$ and is tilted with respect to the scattering plane by $\chi = \frac{1}{2} \arctan \frac{P_2}{P_1}$.

C. Stokes parameters of scattered light

By inserting the parametrization of the density matrix (9) into Eq. (8), we can relate the Stokes parameters of the incoming and scattered photons for a closed-shell system:

$$P_{1f} = \frac{|S|^2(P_{1i}+1) - (1-P_{1i})}{|S|^2(P_{1i}+1) + (1-P_{1i})}, \quad (10)$$

$$P_{2f} = \frac{2P_{2i}\,\mathrm{Re}\,(S) + 2P_{3i}\,\mathrm{Im}\,(S)}{|S|^2(P_{1i}+1) + (1-P_{1i})}, \quad (11)$$

$$P_{3f} = \frac{2P_{3i}\,\mathrm{Re}\,(S) - 2P_{2i}\,\mathrm{Im}\,(S)}{|S|^2(P_{1i}+1) + (1-P_{1i})}. \quad (12)$$

Here, the indices i and f denote the Stokes parameters of the initial and final photons and S is the amplitude ratio (6). We remind the reader that the Stokes parameters P_1 and P_2, which describe the linear polarization, are defined with respect to the scattering plane, characterized by the momenta $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$.

Equations (10)–(12) describe the most general case when the polarization of incoming and outgoing photons are characterized by all three Stokes parameters. In today's experiments, however, not all of these parameters can be observed. In typical synchrotron studies, for example, the incident photons are linearly polarized within the synchrotron plane and only linear polarization of scattered light can be measured. In the next section, we discuss how Eqs. (10)–(12) can be adapted for this synchrotron scenario.

IV. DETAILS OF CALCULATIONS

The relations between the Stokes parameters of the incoming and outgoing photons (10)–(12) are general and hold true for any closed-shell system. However, to calculate the particular values of the polarization parameters we have to evaluate the amplitude ratio S. As seen from Eqs. (1), (6), and (8), the calculation of the matrix elements M_{fi} requires the summation over the intermediate states $|\alpha_\nu J_\nu M_\nu\rangle$. This summation runs over the entire spectrum of the many-electron atom, including the positive and negative continua. For many-electron systems, this summation can be carried out only approximately by using various approximative methods. In the present study, we use the independent-particle approximation (IPA), in which the photon interacts with a single active electron, while the other electrons remain frozen. During the last decades, the IPA model has been successfully applied to describe Rayleigh scattering off closed-shell atoms for which $J_f = J_i = 0$ and $M_i = M_f = 0$ [2,17]. For such a closed-shell system, the many-electron-scattering amplitude can be written within the IPA as

$$M_{fi}(\boldsymbol{k}_1, \chi_1, \boldsymbol{k}_2, \chi_2) = \sum_{njlm} M_{njlm}(\boldsymbol{k}_1, \chi_1, \boldsymbol{k}_2, \chi_2), \quad (13)$$

where the summation runs over all occupied single electron states. These states are described by the principle quantum number n, the total and angular momenta j and l, and where the projection of the total angular momentum m in the initial and final states is the same. For the sake of brevity, we do not discuss the evaluation of the one-electron matrix element M_{njlm} and refer to the literature [1,3,18–22].

V. RESULTS AND DISCUSSION

In this section, we apply the general expressions (10)–(12) to analyze the polarization transfer between incident and outgoing photons for the typical setup of a synchrotron experiment. In this setup, the incident photons are almost completely linearly polarized within the synchrotron plane and the detectors can only measure the linear polarization of the scattered photons. Therefore, we assume $P_{3i} = 0$ and focus on the first and second Stokes parameter of the scattered light:

$$P_{1f} = \frac{|S|^2[1 + P_{l,i}\cos(2\varphi)] - [1 - P_{l,i}\cos(2\varphi)]}{|S|^2[1 + P_{l,i}\cos(2\varphi)] + [1 - P_{l,i}\cos(2\varphi)]}, \quad (14)$$

$$P_{2f} = \frac{2P_{l,i}\sin(2\varphi)\,\mathrm{Re}\,(S)}{|S|^2[1 + P_{l,i}\cos(2\varphi)] + [1 - P_{l,i}\cos(2\varphi)]}. \quad (15)$$

These expressions are obtained from Eqs. (10) and (11), in which the parameters of the polarization ellipse are used instead of the initial-state Stokes parameters P_{1i} and P_{2i} and the tilt angle with respect to the scattering plane of the semimajor axis of this ellipse is given by $\chi = \varphi$, see Fig. 1.

Despite the naive expectation that synchrotron radiation is completely linearly polarized if emitted within the synchrotron plane, this is not the case under real conditions. For example, a small depolarization $\delta_i = 1 - P_{l,i} \ll 1$ of x rays emitted from PETRA III facility at DESY has been reported recently in Refs. [10,11]. The determination of δ_i remains for the moment a theoretical and experimental challenge. Recently, it was proposed to determine δ_i from the measurements of the linear polarization of the scattered photons [10]. The outcome of these measurements depends on the azimuthal angle φ under which the scattered photons are detected. For example, in the experiment by Blumenhagen and coworkers [11], the detector was placed within the synchrotron plane, i.e., at $\varphi = 0^\circ$. In this case Eqs. (14) and (15) can be simplified to

$$P_{1f}(\varphi = 0^\circ) = \frac{\frac{|S|^2-1}{|S|^2+1} + (1-\delta_i)}{1 + \frac{|S|^2-1}{|S|^2+1}(1-\delta_i)} = 1 - \frac{2}{1 + \frac{2-\delta_i}{\delta_i}|S|^2}, \quad (16)$$

$$P_{2f}(\varphi = 0^\circ) = 0, \quad (17)$$

as was already shown in Ref. [10]. These formulas indicate that the depolarization δ_i can be determined from measuring the Stokes parameter $P_{1f}(\varphi = 0^\circ)$, if the amplitude ratio S is known from theoretical calculations. As already mentioned above, however, the evaluation of S is a very complicated task and can be performed only approximately. Therefore, the calculation of the second-order amplitudes can introduce additional uncertainties to the determination of the polarization purity of synchrotron radiation.

To avoid theoretical uncertainties in the analysis of the polarization purity of synchrotron radiation, we propose to extend the previous measurement scheme in such a way that δ_i is determined based solely on the experimental data. This new scenario requires us to measure the linear polarization of the photons, scattered not only within the synchrotron plane,

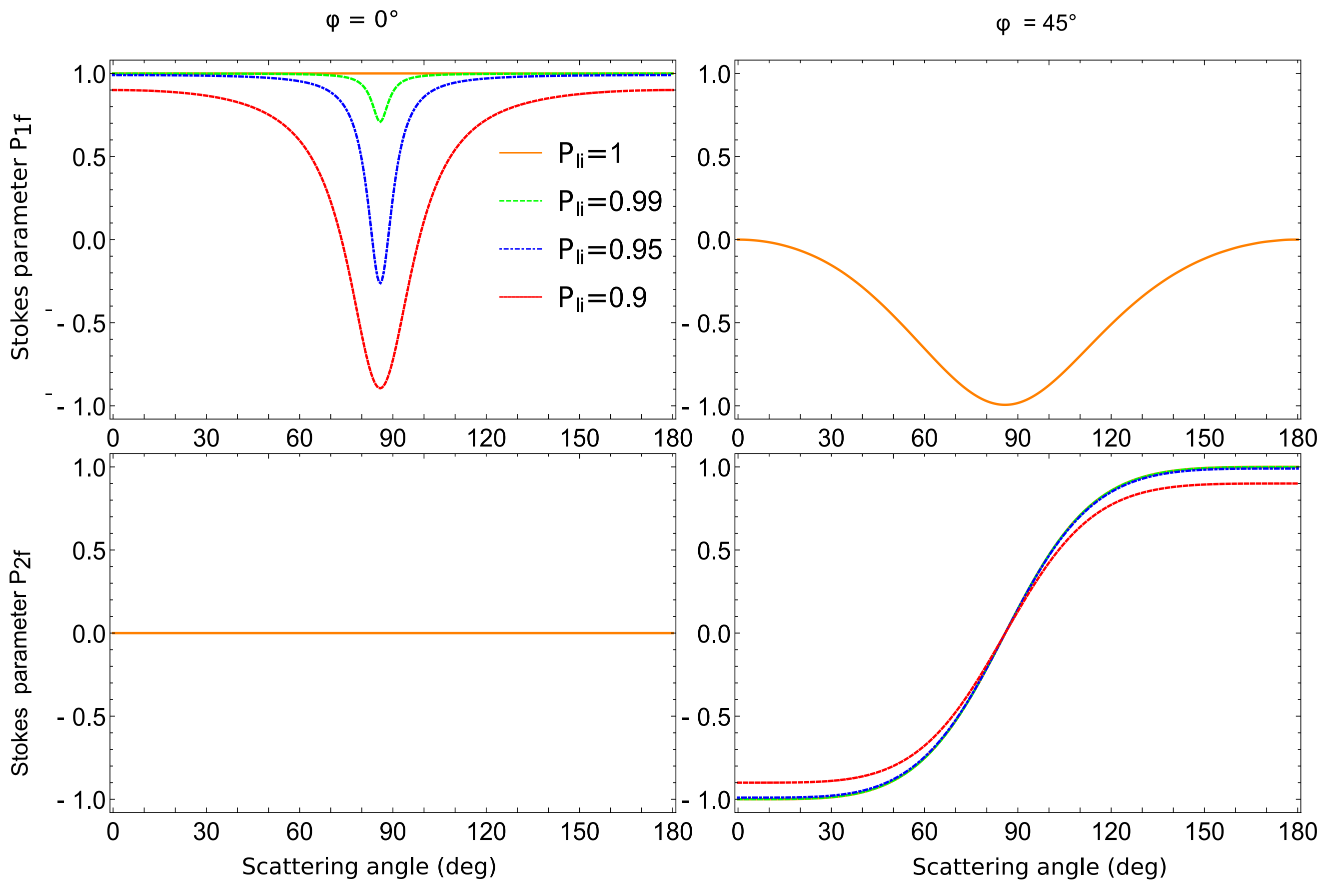

FIG. 2. The Stokes parameters of the scattered radiation P_{1f} and P_{2f} depending on the scattering angle θ, for different degrees of linear polarization of the incoming radiation $P_{l,i}$ and different azimuthal angles φ for scattering of 145 keV x rays off a lead atom (Pb, $Z = 82$). The results of $P_{1f}(\varphi = 45^\circ)$ and $P_{2f}(\varphi = 0^\circ)$ for different initial depolarizations coincide as predicted by Eqs. (17) and (18).

$\varphi = 0^\circ$, but also at the azimuthal angle $\varphi = 45^\circ$. For the latter case, Eqs. (14) and (15) can be written as

$$P_{1f}(\varphi = 45^\circ) = \frac{|S|^2 - 1}{|S|^2 + 1}, \tag{18}$$

$$P_{2f}(\varphi = 45^\circ) = \frac{2\,\mathrm{Re}\,(S)(1 - \delta_i)}{|S|^2 + 1}. \tag{19}$$

As seen from these expressions, the Stokes parameter $P_{1f}(\varphi = 45^\circ)$ is independent of the polarization of incident light and is defined just by the amplitude ratio S. We can therefore combine Eqs. (16) and (18) in order to exclude the ratio S and determine the depolarization:

$$\delta_i = 1 - \frac{P_{1f}(\varphi = 0^\circ) - P_{1f}(\varphi = 45^\circ)}{1 - P_{1f}(\varphi = 0^\circ)P_{1f}(\varphi = 45^\circ)}. \tag{20}$$

This expression clearly shows that the parameter δ_i can be obtained without any need for theoretical data, if the scattered photons are observed by polarization-sensitive detectors within the synchrotron plane and under the angle 45° for the same target, photon energy, and polar scattering angle. Furthermore, Eq. (20) is obtained based on Eq. (10), which is in general independent of P_{3i}, and hence the precision in the determination of δ_i by measuring the polarization of the scattered light at the angles $\varphi = 0^\circ$ and $\varphi = 45^\circ$ is not affected by circular polarization of the incident photon.

To discuss the feasibility of the polarization analysis based on Eq. (20), we present results for a typical synchrotron experiment in Fig. 2. The calculations have been performed for 145 keV photons scattered off lead atoms and the summation in Eq. (13) was restricted to the K, L, M, and N shells. The contributions of the O and P shells were not included in our analysis because they are known to affect the polarization properties only for very small scattering angles $\theta \leqslant 5^\circ$ [10], which are not available for experimental observation. We note that our results for the scattering amplitudes are in perfect agreement with Ref. [3].

In our calculations, we assume that the incident light is either completely linearly polarized or slightly depolarized with the parameter $\delta_i = 0.01,\ 0.05,\ 0.1$. As seen from Fig. 2, a high sensitivity to this depolarization is exhibited by the Stokes parameter P_{1f}, when measured within the synchrotron plane, i.e., $\varphi = 0^\circ$. These results are consistent with previous theoretical and experimental data and, moreover, indicate that the depolarization effect is most pronounced for the polar scattering angles close to $\theta \approx 90^\circ$ [10,11]. For example, the parameter $P_{1f}(\varphi = 0^\circ, \theta \approx 90^\circ)$ decreases from 1 to 0.7, if the polarization of incident light is reduced only slightly from 100% to 99%. One would conclude that the analysis of the polarization purity of synchrotron radiation, based on Eq. (20), can be performed most conveniently for $\theta \approx 90^\circ$. These angles also favor the measurement of the Stokes parameter

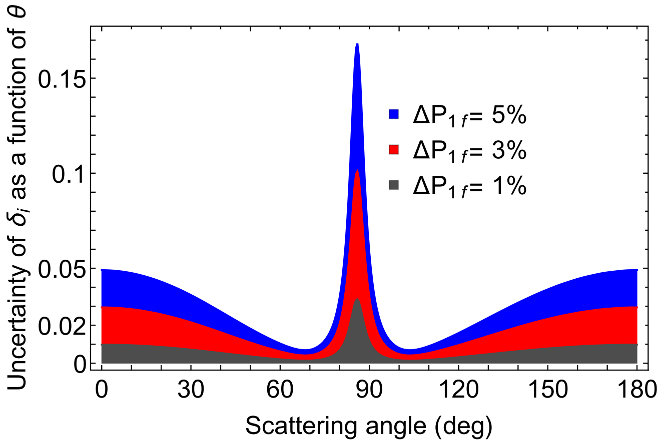

FIG. 3. Initial depolarization $\delta_i = 0.02$ determined through theoretical calculations of $P_{1f}(\varphi = 0^\circ)$ and $P_{1f}(\varphi = 45^\circ)$ with initial photon energy of 145 keV scattered by a lead atom. The gray, red, and blue shadowed areas show the angular-dependent uncertainty in the determination of δ_i for a relative uncertainty of 1%, 3%, and 5% in the measurements of P_{1f}.

$P_{1f}(\varphi = 45^\circ)$, whose absolute values reach their maximum for the photons emitted perpendicularly to the incident-beam axis. However, this expectation about the advantage of the scattering angles $\theta \approx 90^\circ$ for the polarization purity analysis did not take into account measurement uncertainties. For instance, in the recent experiment performed for 175 keV x rays scattered off gold atoms, the polarization was determined with an uncertainty in the range from 3% to 12% depending on the polar scattering angle [11]. To study how such uncertainties may affect the accuracy of the polarization purity analysis (20), we derived the absolute error in the determination of δ_i:

$$\Delta\delta_i = \left\{\left[\frac{\partial\delta_i}{\partial P_{1f}(\varphi = 0^\circ)}\right]^2 \Delta P_{1f}^2(\varphi = 0^\circ) + \left[\frac{\partial\delta_i}{\partial P_{1f}(\varphi = 45^\circ)}\right]^2 \Delta P_{1f}^2(\varphi = 45^\circ)\right\}^{\frac{1}{2}}. \quad (21)$$

In this expression, ΔP_{1f} are the polarization measurement uncertainties. The partial derivatives of δ_i can be obtained with Eq. (20):

$$\frac{\partial\delta_i}{\partial P_{1f}(\varphi = 0^\circ)} = \frac{P_{1f}^2(\varphi = 45^\circ) - 1}{[P_{1f}(\varphi = 0^\circ)P_{1f}(\varphi = 45^\circ) - 1]^2}, \quad (22)$$

$$\frac{\partial\delta_i}{\partial P_{1f}(\varphi = 45^\circ)} = \frac{1 - P_{1f}^2(\varphi = 0^\circ)}{[P_{1f}(\varphi = 0^\circ)P_{1f}(\varphi = 45^\circ) - 1]^2}. \quad (23)$$

By making use of these expressions, we can analyze the feasibility of the polarimetry scheme for the determination of the polarization purity of synchrotron radiation. We performed calculations of 145 keV photons with initial depolarization $\delta_i = 0.02$, scattered off lead atoms, assuming different uncertainties for the Stokes parameters P_{1f}. In Fig. 3, we show the uncertainty in the determination of δ_i. We have assumed that the Stokes parameters of scattered photons are measured with a relative uncertainty of $\Delta P_{1f}/P_{1f} =$ 1%, 3%, 5%. These experimental uncertainties are displayed by gray, red, and blue shaded areas, respectively. As seen from this figure, $\Delta\delta_i$ is very sensitive to the polar scattering angle and reaches its maximum at $\theta \approx 90^\circ$. We conclude, therefore, that despite of the high polarization sensitivity of $P_{1f}(\varphi = 0^\circ, \theta \approx 90^\circ)$ and of large values of $P_{1f}(\varphi = 45^\circ, \theta \approx 90^\circ)$, the implementation of the scheme, based on Eq. (20), for the photons emitted perpendicularly to the incident-beam direction, is impractical. In contrast, as one can conclude from Figs. 2 and 3, the scattering angles 70° and 105° can be very convenient for the polarization measurements. For these angles $P_{1f}(\varphi = 0)$ and $P_{1f}(\varphi = 45^\circ)$ are still large and can be easily measured, and, moreover, $\Delta\delta_i$ is small. For example, our calculations indicate that Eqs. (20) and (21), if applied for $\theta = 70^\circ$, predict $\delta_i = 0.020 \pm 0.001$ for the experimental uncertainty of 1% and $\delta_i = 0.020 \pm 0.006$ for $\Delta P_{1f} = 4\%$. We note that the relative experimental uncertainty of 4% has already been realized experimentally at the polar scattering angle $\theta = 65^\circ$ [11].

So far, we have discussed the feasibility of simultaneous measurements of the scattered photons at the azimuthal angles $\varphi = 0^\circ$ and $\varphi = 45^\circ$ for the polarization purity diagnostics of synchrotron radiation for the particular case of 145 keV photons interacting with a lead target. To explore whether Eq. (20) can be applied for other energies and targets we have performed detailed calculations for x rays in the region of 100 to 500 keV and for various heavy atoms. The results of these calculations have shown that the qualitative behavior of $P_{1f}(\varphi = 0)$ and $P_{1f}(\varphi = 45^\circ)$, as well as of the uncertainty $\Delta\delta_i$ is rather insensitive to the photon energy and the nuclear target and resemble the results displayed in Figs. 2 and 3. For the sake of brevity, these results are not displayed in this article.

VI. SUMMARY

In summary, we re-investigated the Rayleigh scattering of x rays by closed-shell atoms. We found general formulas for the Stokes parameters of the scattered photons, depending on the initial Stokes parameters and the second-order scattering amplitudes. We suggest using these formulas to investigate the polarization purity of synchrotron radiation. In contrast with previous works, our proposal does not rely on theoretical calculations of the second-order many-electron amplitudes. Taking into account measurement uncertainties, we propose a polarimetry scheme, where $P_{1f}(\varphi = 0^\circ)$ and $P_{1f}(\varphi = 45^\circ)$ measured at the scattering angle 70° or 105°. For this scenario, we predict the least uncertainty in the determination of the initial depolarization. This Rayleigh polarimetry is likely to be realized soon at the PETRA III facility at DESY. We expect a deeper insight into the polarization of synchrotron radiation.

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