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Spin-polarization after scattering

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ABSTRACT

This paper deals with the spin-polarization change of an electron beam after elastic scattering with a neutral atom. The first part of the paper is devoted to summarizing the Kessler theory of the elastic scattering of spin-polarized electron beams. After a general description of the dependence on the polar and azimuthal angles of the spin-polarization after scattering, the effects on the spin-polarization of multiple elastic collisions occurring in the same scattering plane and with identical scattering angles are also treated. In particular, we show that, in this case, an initially unpolarized beam becomes fully polarized in the direction normal to the scattering plane after a number of collisions. The number of collisions necessary to reach full (transverse) polarization is a function of the common scattering angle. We also demonstrate that spin-polarization is conserved for forward and backward elastic scattering.

1. Introduction

This paper deals with the study of the spin-polarization change of electron beams due to the elastic scattering with neutral atoms [1].

A quantum system with two quantum states represents a quantum bit, or qubit [2]. Among the many applications of qubits, let us mention quantum cryptography. It provides information security by using quantum channels. Quantum key distribution, discussed by Wiesner [3], represents, for example, a quantum cryptographic protocol ensuring the secrecy of a key constituted by a sequence of binary digits. The quantum information theory deals with quantum noise in order to protect physical qubits from its effects. It is important to be able to model and control quantum noise.

Quantum information is independent of the physical systems used to implement qubits, as any two-state quantum system can represent a qubit [4]. In particular, the spin of an electron can be used to implement a qubit.

An electron beam is a quantum system in a mixed state of spin orientations. It is said to be polarized when the electron spins have a preferential orientation.

A set of observable quantities, the polarization parameters S, T, and U, can be defined. They depend on the scattering angle and on the incident electron kinetic energy. The final polarization after an elastic scattering collision is a function of these polarization parameters.

In the following, we will discuss the spin-polarization change of an electron beam after elastic scattering.

The paper is organized as follows: The Kessler theory of the elastic scattering of spin-polarized electron beams is first briefly summarized in Section 2. Then, in Section 3, we discuss spin-polarization after scattering. In Section 3.1 we consider the dependence on the polar and azimuthal angles of the spin-polarization after scattering. We are interested, in particular, in multiple collisions, i.e., a sequence of elastic collisions. The spin-polarization changes after every collision. We describe how to calculate the spin-polarization of the beam after any elastic collision in the sequence in Section 3.2. In Section 3.3 we consider, in particular, the special case of a sequence of collisions occurring in the same plane of scattering. In Section 3.4, the even more special case of a sequence of elastic collisions occurring in the same plane and with the same scattering angle is investigated. We then demonstrate, in Section 3.5, that, in such a case, an initially unpolarized beam approaches full (transverse) spin-polarization after a number of elastic collisions which depends on the target atom, the initial energy, and the scattering angle ϑ. In the concluding Section 3.6, we demonstrate the conservation of spin-polarization for forward and backward elastic scattering.

2. The theory of the elastic scattering of spin-polarized electron beams

Partially polarized electron beams (positron beams) are mixed spin states, i.e., they are statistical mixtures of pure spin states. Thus, according to Kessler, it helps to describe them using the formalism of the density matrix [1]. For a statistical mixture of pure spin states, the

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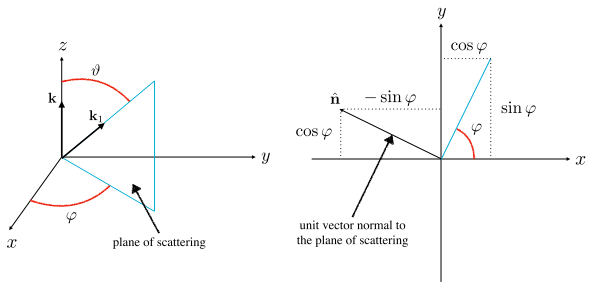

Fig. 1. Scattering geometry. The illustration indicates the definition of the scattering plane. z axis is oriented along the direction of electron incidence. $\mathbf{k}$ is the electron momentum before scattering, $\mathbf{k}_1$ is the electron momentum after scattering, ϑ is the scattering angle, and φ is the azimuthal angle. The unit vector $\hat{\mathbf{n}}$ perpendicular to the plane of scattering is given by $(\mathbf{k}\times\mathbf{k}_1)/|\mathbf{k}\times\mathbf{k}_1|$.

density matrix ρ is given by

$$\rho = \frac{1}{2}(I + \boldsymbol{\sigma}\cdot\mathbf{P}) = \frac{1}{2}\begin{pmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{pmatrix}, \tag{1}$$

where $\mathbf{P}$ is the initial spin-polarization, i.e., the spin-polarization of the beam before scattering,

$$\mathbf{P} = \begin{pmatrix} P_x \\ P_y \\ P_z \end{pmatrix}, \tag{2}$$

and $\boldsymbol{\sigma}$ is the vector

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} \tag{3}$$

whose components σ_x, σ_y, and σ_z are the Pauli matrices.[1] The density matrix and the polarization are connected by the relationship

$$\mathbf{P} = \langle\boldsymbol{\sigma}\rangle = \mathrm{Tr}(\rho\boldsymbol{\sigma}), \tag{5}$$

or

$$P_i = \mathrm{Tr}(\rho\sigma_i), \tag{6}$$

where $i = 1,2,3$, $P_1 = P_x$, $P_2 = P_y$, $P_3 = P_z$, $\sigma_1 = \sigma_x$, $\sigma_2 = \sigma_y$, and $\sigma_3 = \sigma_z$.

Let us choose the z axis along the direction of electron/positron incidence and introduce the scattering matrix F for the spin:

$$F = \begin{pmatrix} f(\vartheta) & -g(\vartheta)\,e^{-i\varphi} \\ g(\vartheta)\,e^{i\varphi} & f(\vartheta) \end{pmatrix}, \tag{7}$$

where φ is the azimuthal angle, ϑ is the polar angle, $f(\vartheta)$ is the direct scattering amplitude, and $g(\vartheta)$ is the spin-flip scattering amplitude. Please note that

$$\begin{aligned} FF^\dagger &= F^\dagger F = \\ &= \begin{pmatrix} f & -g\,e^{-i\varphi} \\ g\,e^{i\varphi} & f \end{pmatrix}\begin{pmatrix} f^* & g^*\,e^{-i\varphi} \\ -g^*\,e^{i\varphi} & f^* \end{pmatrix} = \\ &= \begin{pmatrix} f^* & g^*\,e^{-i\varphi} \\ -g^*\,e^{i\varphi} & f^* \end{pmatrix}\begin{pmatrix} f & -g\,e^{-i\varphi} \\ g\,e^{i\varphi} & f \end{pmatrix} = \\ &= \begin{pmatrix} |f|^2+|g|^2 & (fg^*-f^*g)e^{-i\varphi} \\ -(fg^*-f^*g)e^{i\varphi} & |f|^2+|g|^2 \end{pmatrix}. \end{aligned} \tag{8}$$

The mean value of $FF^\dagger = F^\dagger F$ is the trace of $\rho FF^\dagger$

$$\langle FF^\dagger\rangle = \mathrm{Tr}(\rho FF^\dagger) = \mathrm{Tr}(\rho F^\dagger F) = \mathrm{Tr}(F\rho F^\dagger) \tag{9}$$

and represents the differential elastic scattering cross-section $d\sigma(\vartheta,\varphi)/d\Omega$, where $d\Omega$ is the differential of the solid angle,

$$d\Omega = \sin\vartheta d\vartheta\, d\varphi\,. \tag{10}$$

We thus have

$$\begin{aligned} \frac{d\sigma(\vartheta,\varphi)}{d\Omega} &= \langle FF^\dagger\rangle = \mathrm{Tr}(\rho FF^\dagger) = \\ &= \frac{1}{2}\mathrm{Tr}\left[\begin{pmatrix} 1+P_z & P_x-iP_y \\ P_x+iP_y & 1-P_z \end{pmatrix}\begin{pmatrix} |f|^2+|g|^2 & (fg^*-f^*g)e^{-i\varphi} \\ -(fg^*-f^*g)e^{i\varphi} & |f|^2+|g|^2 \end{pmatrix}\right] = \\ &= (|f|^2+|g|^2)[1 - S(\vartheta)(P_x\sin\varphi - P_y\cos\varphi)], \end{aligned} \tag{11}$$

where we have introduced the Sherman function $S(\vartheta)$ given by

$$S(\vartheta) = i\frac{f(\vartheta)g^*(\vartheta) - f^*(\vartheta)g(\vartheta)}{|f(\vartheta)|^2+|g(\vartheta)|^2}. \tag{12}$$

If we indicate with $\hat{\mathbf{n}}$ the unit vector perpendicular to the plane of scattering (see Fig. 1),

$$\hat{\mathbf{n}} = \hat{\mathbf{n}}(\varphi) = \begin{pmatrix} -\sin\varphi \\ \cos\varphi \\ 0 \end{pmatrix}, \tag{13}$$

from Eq. (11) we have

$$\frac{d\sigma(\vartheta,\varphi)}{d\Omega} = (|f|^2+|g|^2)[1 + S(\vartheta)\mathbf{P}\cdot\hat{\mathbf{n}}]. \tag{14}$$

After an elastic scattering, the statistical mixture of the beam spin states changes. The transformation of the density matrix ρ can be obtained using the scattering matrix F for the spin. Note that the transformed density matrix $F\rho F^\dagger$ has to be normalized, in order to make its trace equal to 1. The final density matrix ρ^f (density matrix after scattering) is thus given by

$$\rho^f = \frac{F\rho F^\dagger}{\mathrm{Tr}(F\rho F^\dagger)}, \tag{15}$$

We can now calculate the spin-polarization vector $\mathbf{P}^f$ after scattering. If $\mathbf{P}$ is the spin-polarization vector before scattering, then

$$\mathbf{P}^f = \mathrm{Tr}(\rho^f\boldsymbol{\sigma}) = \frac{\mathrm{Tr}(F\,F^\dagger\boldsymbol{\sigma}) + \mathrm{Tr}(F\,(\boldsymbol{\sigma}\cdot\mathbf{P})\,F^\dagger\boldsymbol{\sigma})}{\mathrm{Tr}(F\,F^\dagger) + \mathrm{Tr}(F\,(\boldsymbol{\sigma}\cdot\mathbf{P})\,F^\dagger)}. \tag{16}$$

Let us observe that

$$\mathrm{Tr}(F\,F^\dagger) = 2\,(|f|^2 + |g|^2), \tag{17}$$

$$\mathrm{Tr}(F\,F^\dagger\boldsymbol{\sigma}) = 2\,i(fg^* - f^*g)\,\hat{\mathbf{n}}, \tag{18}$$

$$\mathrm{Tr}(F\,(\boldsymbol{\sigma}\cdot\mathbf{P})\,F^\dagger) = 2\,i(fg^* - f^*g)\,\mathbf{P}\cdot\hat{\mathbf{n}}, \tag{19}$$

$$\begin{aligned} &\mathrm{Tr}(F\,(\boldsymbol{\sigma}\cdot\mathbf{P})\,F^\dagger\boldsymbol{\sigma}) = \\ &= 2\,(|f|^2 - |g|^2)\mathbf{P} - 2\,(fg^* + f^*g)\,\mathbf{P}\times\hat{\mathbf{n}} + 4|g|^2\,(\mathbf{P}\cdot\hat{\mathbf{n}})\,\hat{\mathbf{n}}. \end{aligned} \tag{20}$$

Let us now introduce the spin-polarization functions $T(\vartheta)$ and $U(\vartheta)$:

$$T(\vartheta) = \frac{|f(\vartheta)|^2 - |g(\vartheta)|^2}{|f(\vartheta)|^2 + |g(\vartheta)|^2}, \tag{21}$$

$$U(\vartheta) = \frac{f(\vartheta)g^*(\vartheta) + f^*(\vartheta)g(\vartheta)}{|f(\vartheta)|^2 + |g(\vartheta)|^2}. \tag{22}$$

Note that

$$S^2(\vartheta) + T^2(\vartheta) + U^2(\vartheta) = 1 \tag{23}$$

and

$$\frac{2\,|g|^2}{|f|^2 + |g|^2} = 1 - T(\vartheta). \tag{24}$$

[1] Note that the density matrix can be diagonalized choosing the z-axis so that $P_x = 0$, $P_y = 0$, $P_z = P$. In fact, is such a case,

$$\rho = \frac{1}{2}\begin{pmatrix} 1+P & 0 \\ 0 & 1-P \end{pmatrix}. \tag{4}$$

From this equation it follows that, if N is the number of measurements with spin up and M the number of measurements with spin down, then the probability of spin up, $N/(N+M)$, is given by $(1+P)/2$ while the probability of spin down, $M/(N+M)$, is given by $(1-P)/2$. Therefore $P = (N-M)/(N+M)$.

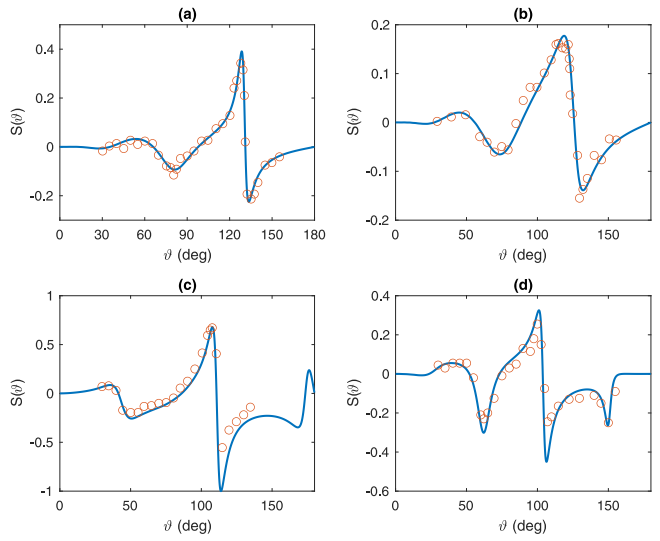

Fig. 2. (a) POLARe2 calculation of the Sherman function of a 900 eV electron beam impinging on Xe neutral atoms (solid line) compared with the Kessler et al. experimental data (symbols) [5]. (b) POLARe2 calculation of the Sherman function of a 1200 eV electron beam impinging on Xe neutral atoms (solid line) compared with the Kessler et al. experimental data (symbols) [5]. (c) POLARe2 calculation of the Sherman function of a 150 eV electron beam impinging on Hg neutral atoms (solid line) compared with the Berger and Kessler experimental data (symbols) [6]. (d) POLARe2 calculation of the Sherman function of 700 eV electron beam impinging on Hg neutral atoms (solid line) compared with the Steidl et al. experimental data (symbols) [7].

3. Results and discussion

Calculations of the scattering parameters presented in this paper were performed using the POLARe2 code [8,9]. The POLARe2 program is based, like the POLARe program, on the solution of the Dirac equation in a central field (Mott theory [10]).[2] The POLARe and POLARe2 codes were validated by comparison with many experimental data and theoretical calculations [11–17]. Other programs are available for the calculation of the scattering parameters, in particular ELSEPA [18, 19]. Both the POLARe and POLARe2 codes use the screening functions proposed by Cox and Bonham [20] (Z=1-54) and by Salvat et al. [21] (Z=55-92). Exchange effects are included in the calculation of the atomic potential energy [22,23] for electron beams. According to Salvat [24], further corrections to the electrostatic potential, i.e., correlation-atomic polarization potential, not included in POLARe, are included in POLARe2: In particular, the Buckingham potential was used to describe long-range polarization for both electrons and positrons [18,24], the Perdew and Zunger theory was used for calculating the short-range polarization potential for electrons [25], and the Jain approach was utilized for calculating short-range polarization potential for positrons [26]. Calculated Sherman functions (for Xe and Hg) are presented in Fig. 2 and compared with experimental data. In Figs. 2(a) and 2(b) we compare the POLARe2 calculation of the Sherman function of electron beams of 900 eV and 1200 eV, respectively, impinging on Xe neutral atoms with the Kessler et al. experimental data [5]. In Fig. 2(c) we present the comparison of the POLARe2 calculations with the Berger and Kessler experimental data [6] concerning a 150 eV electron beam impinging on Hg neutral atoms. In Fig. 2(d), finally, the calculated Sherman function of 700 eV electron beam impinging on Hg neutral atoms is compared with the Steidl et al. experimental data [7].

[2] The POLARe and POLARe2 programs can be obtained free of charge from https://github.com/mauriziodapor/POLARe

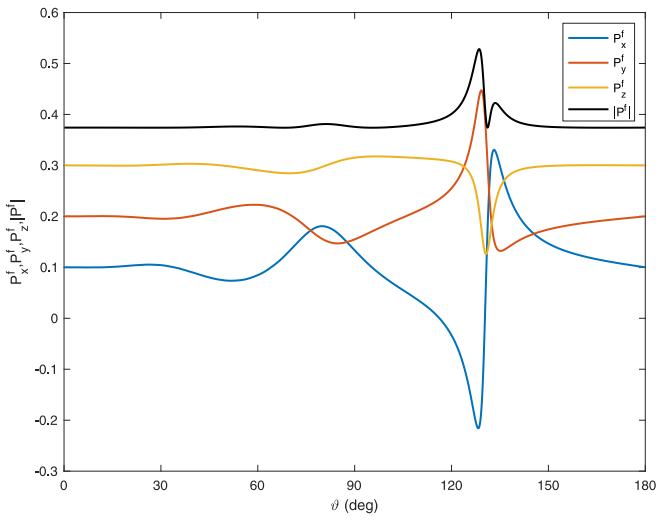

Fig. 3. SPAS calculation of the components and of the modulus of the polarization after the scattering of a 900 eV electron beam impinging on Xe neutral atoms in the laboratory system of reference. Initial polarization: P_x=0.1, P_y=0.2, P_z=0.3. Azimuthal angle: φ=60 deg.

3.1. Spin-polarization after scattering: Dependence on the polar and azimuthal angles

By using Eq. (16), we obtain, in the general case $0 \le |\mathbf{P}| \le 1$, the polarization $\mathbf{P}^f$ of an electron beam or a positron beam after an elastic collision with a neutral atom:

$$\mathbf{P}^f = \frac{[\mathbf{P}\cdot\hat{\mathbf{n}} + S(\vartheta)]\,\hat{\mathbf{n}} + T(\vartheta)[\mathbf{P} - (\mathbf{P}\cdot\hat{\mathbf{n}})\,\hat{\mathbf{n}}] + U(\vartheta)\,(\hat{\mathbf{n}}\times\mathbf{P})}{1 + (\mathbf{P}\cdot\hat{\mathbf{n}})\,S(\vartheta)}\,. \tag{25}$$

It follows from Eq. (25) that the final polarization of an initially unpolarized beam ($\mathbf{P} = 0$) after a single elastic collision is given by

$$\mathbf{P}^f = S(\vartheta)\,\hat{\mathbf{n}}\,. \tag{26}$$

Since

$$\mathbf{P}\cdot\hat{\mathbf{n}} = -P_x \sin\varphi + P_y \cos\varphi\,, \tag{27}$$

we have

$$(\mathbf{P}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}} = \begin{pmatrix} P_x \sin^2\varphi - P_y \sin\varphi\cos\varphi \\ P_y \cos^2\varphi - P_x \sin\varphi\cos\varphi \\ 0 \end{pmatrix}. \tag{28}$$

Furthermore,

$$\hat{\mathbf{n}}\times\mathbf{P} = \begin{pmatrix} P_z\cos\varphi \\ P_z\sin\varphi \\ -P_x\cos\varphi - P_y\sin\varphi \end{pmatrix}. \tag{29}$$

Let us now introduce the quantity $D(\vartheta,\varphi)$, defined as

$$D(\vartheta,\varphi) = 1 + S(\vartheta)(P_y\cos\varphi - P_x\sin\varphi)\,, \tag{30}$$

so that, if

$$\mathbf{P}^f = \begin{pmatrix} P_x^f \\ P_y^f \\ P_z^f \end{pmatrix}, \tag{31}$$

we have

$$P_x^f = \frac{1}{D(\vartheta,\varphi)}[P_x\sin^2\varphi - P_y\sin\varphi\cos\varphi - S(\vartheta)\sin\varphi + \\ + T(\vartheta)P_x\cos^2\varphi + T(\vartheta)P_y\sin\varphi\cos\varphi + U(\vartheta)P_z\cos\varphi]\,, \tag{32}$$

$$P_y^f = \frac{1}{D(\vartheta,\varphi)}[P_y\cos^2\varphi - P_x\sin\varphi\cos\varphi + S(\vartheta)\cos\varphi +$$

$$+T(\vartheta)P_y\sin^2\varphi + T(\vartheta)P_x\sin\varphi\cos\varphi + U(\vartheta)P_z\sin\varphi]\,, \tag{33}$$

$$P_z^f = \frac{1}{D(\vartheta,\varphi)}[T(\vartheta)P_z - U(\vartheta)(P_x\cos\varphi + P_y\sin\varphi)]\,. \tag{34}$$

In Fig. 3 we present the components of the spin-polarization after scattering, $\mathbf{P}^f$, (in the laboratory system of reference) as a function of the scattering angle ϑ for the case in which the components of the initial spin-polarization (in the laboratory system of reference) are $P_x = 0.1$, $P_y = 0.2$, $P_z = 0.3$, the azimuthal angle is $\varphi = 60$ deg, the target atom is Xe, and the electron kinetic energy is 900 eV. In the same Fig. 3, the square root of the sum of the squares of these components, i.e., the modulus of the spin polarization, is represented. The SPAS program (Spin-Polarization After Scattering)[3] allows calculating the spin-polarization of electron and positron beams after scattering with any set of initial conditions. It requires in input the functions $S(\vartheta)$, $T(\vartheta)$, and $U(\vartheta)$ (which can be obtained using POLARe or POLARe2 [9], or any other software able to calculate the scattering amplitudes $f(\vartheta)$ and $g(\vartheta)$ such as, for example, ELSEPA [18,19]).

Let us now consider a few quite simple and useful particular cases. First of all, if the initial spin-polarization is null then $D(\vartheta,\varphi) = 1$ and, as already observed [see Eq. (26)], we have

$$P_x^f = -S(\vartheta)\sin\varphi\,, \tag{35}$$

$$P_y^f = S(\vartheta)\cos\varphi\,, \tag{36}$$

$$P_z^f = 0\,. \tag{37}$$

Hence, in this case, the modulus of the spin-polarization after scattering is given by the absolute value of the Sherman function $S(\vartheta)$ (also known, for this reason, as the spin-polarization function):

$$|\mathbf{P}^f| = |S(\vartheta)|\,. \tag{38}$$

If the direction of the spin-polarization $\mathbf{P}$ before scattering is the direction of electron incidence, i.e., if $P_x = P_y = 0$ and $P_z \neq 0$ (longitudinal initial spin-polarization), we still have $D(\vartheta,\varphi) = 1$ and

$$P_x^f = -S(\vartheta)\sin\varphi + U(\vartheta)P_z\cos\varphi\,, \tag{39}$$

$$P_y^f = S(\vartheta)\cos\varphi + U(\vartheta)P_z\sin\varphi\,, \tag{40}$$

$$P_z^f = T(\vartheta)P_z\,. \tag{41}$$

The modulus of the spin-polarization after scattering is given, in this case, by

$$|\mathbf{P}^f| = \sqrt{S(\vartheta)^2 + [T(\vartheta)^2 + U(\vartheta)^2]\,P_z^2} = \\ = \sqrt{S(\vartheta)^2 + [1 - S(\vartheta)^2]P_z^2}\,, \tag{42}$$

so that, if $P_x = 0$, $P_y = 0$, $P_z = 1$ and, as a consequence, $|\mathbf{P}| = 1$, then

$$|\mathbf{P}^f| = \sqrt{S(\vartheta)^2 + 1 - S(\vartheta)^2} = 1\,. \tag{43}$$

This is a special case of a general result which can be directly deduced from Eq. (25): If $|\mathbf{P}| = 1$ then $|\mathbf{P}^f| = 1$ [1].

When the primary electron beam is spin-polarized in the transverse direction, e.g., when $P_x \neq 0$, $P_y = 0$, $P_z = 0$, so that it is not axially symmetric with respect to the direction of incidence, we have

$$D(\vartheta,\varphi) = 1 - S(\vartheta)\,P_x\sin\varphi\,, \tag{44}$$

and

$$P_x^f = \frac{P_x\sin^2\varphi - S(\vartheta)\sin\varphi + T(\vartheta)P_x\cos^2\varphi}{D(\vartheta,\varphi)}\,, \tag{45}$$

$$P_y^f = \frac{S(\vartheta)\cos\varphi + [T(\vartheta) - 1]\,P_x\sin\varphi\cos\varphi}{D(\vartheta,\varphi)}\,, \tag{46}$$

$$P_z^f = -\frac{U(\vartheta)P_x\cos\varphi}{D(\vartheta,\varphi)}\,. \tag{47}$$

3.2. Multiple collisions

Let us consider now a sequence of elastic collisions. The spin-polarization changes after every collision. Let us indicate with $\mathbf{P}_m$ the spin-polarization of the beam after the mth collision. Let us assume that the beam be initially unpolarized, i.e., the density matrix is initially given by

$$\rho = \frac{1}{2}I = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \tag{48}$$

and $\mathbf{P}_0 = 0$. We already know that, after the first elastic collision, the beam becomes spin-polarized. If ϑ_1 is the scattering angle, then the spin-polarization after scattering is

$$\mathbf{P}_1 = S(\vartheta_1)\,\hat{\mathbf{n}}_1\,, \tag{49}$$

where S is the Sherman function and $\hat{\mathbf{n}}_1$ is the unit vector normal to the plane of scattering. Using Eq. (25) we can now write the spin-polarization $\mathbf{P}_2$ of the beam after the second elastic collision

$$\mathbf{P}_2 = \frac{[S(\vartheta_1)\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2 + S(\vartheta_2)]\hat{\mathbf{n}}_2 + T(\vartheta_2)\{S(\vartheta_1)\hat{\mathbf{n}}_1 - [S(\vartheta_1)\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2]\hat{\mathbf{n}}_2\} + U(\vartheta_2)\hat{\mathbf{n}}_2\times\hat{\mathbf{n}}_1 S(\vartheta_1)}{1 + S(\vartheta_1)S(\vartheta_2)\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2}\,, \tag{50}$$

where ϑ_2 is the second scattering angle and $\hat{\mathbf{n}}_2$ is the unit vector normal to the second plane of scattering. Proceeding in this way it is possible to calculate the spin-polarization of the beam after any elastic collision in the sequence.

3.3. Collisions in the same plane of scattering

It is also convenient to consider the special case in which the planes of scattering do not change, i.e., we are selecting the collisions occurring in the same plane. In other words, let us focus our attention on the particular collisions with the same azimuthal angle $\varphi = 0$, so that

$$\hat{\mathbf{n}}_1 = \hat{\mathbf{n}}_2 = \hat{\mathbf{n}}\,. \tag{51}$$

In this case, we have

$$\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2 = \cos\psi = 1\,, \tag{52}$$

$$\hat{\mathbf{n}}_1\times\hat{\mathbf{n}}_2 = \sin\psi = 0\,, \tag{53}$$

where we have indicated with ψ the angle between the normals $\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}_2$ to the scattering planes, i.e., the angle between the scattering planes. Of course, we have, in this case,

$$S(\vartheta_1)\hat{\mathbf{n}}_1 - [S(\vartheta_1)\hat{\mathbf{n}}_1\cdot\hat{\mathbf{n}}_2]\hat{\mathbf{n}}_2 = S(\vartheta_1)(\hat{\mathbf{n}}_1 - \hat{\mathbf{n}}_2) = 0\,, \tag{54}$$

so that also $\mathbf{P}_2$ is normal to the plane of scattering and is given by

$$\mathbf{P}_2 = \frac{S(\vartheta_1) + S(\vartheta_2)}{1 + S(\vartheta_1)\,S(\vartheta_2)}\hat{\mathbf{n}}\,. \tag{55}$$

[3] The SPAS program can be obtained free of charge from https://github.com/mauriziodapor/POLARe

Table 1
Spin-polarization of an initially unpolarized electron beam as a function of the number of elastic collisions. The first column represents the number of collisions, while the other columns refer to five different values of the Sherman function (0.1, 0.3, 0.5, 0.7, 0.9). The plane of scattering and the scattering angle are assumed here to be identical for all the sequence of elastic collisions.

m	$S = 0.1$	$S = 0.3$	$S = 0.5$	$S = 0.7$	$S = 0.9$
1	0.100	0.300	0.500	0.700	0.900
2	0.198	0.550	0.800	0.940	0.994
3	0.292	0.730	0.929	0.989	1.000
4	0.381	0.845	0.976	0.998	1.000
5	0.463	0.913	0.992	1.000	1.000
6	0.538	0.952	0.997	1.000	1.000
7	0.606	0.974	0.999	1.000	1.000
8	0.666	0.986	1.000	1.000	1.000
9	0.718	0.992	1.000	1.000	1.000
10	0.763	0.996	1.000	1.000	1.000
20	0.964	1.000	1.000	1.000	1.000
30	0.995	1.000	1.000	1.000	1.000
40	0.999	1.000	1.000	1.000	1.000

3.4. Collisions in the same plane of scattering with identical scattering angles

If we choose, in particular, $\vartheta_1 = \vartheta_2 = \vartheta$, i.e., select identical scattering angles, then

$$\mathbf{P}_2 = \frac{2S(\vartheta)}{1+S^2(\vartheta)}\hat{\mathbf{n}}. \tag{56}$$

Let us now consider a third collision in the same scattering plane and with the same scattering angle ϑ. We have

$$\mathbf{P}_3 = \frac{\mathbf{P}_2\cdot\hat{\mathbf{n}}+S(\vartheta)}{1+(\mathbf{P}_2\cdot\hat{\mathbf{n}})\,S(\vartheta)}\hat{\mathbf{n}}, \tag{57}$$

or

$$\mathbf{P}_3 = \frac{3+S^2(\vartheta)}{1+3S^2(\vartheta)}S(\vartheta)\hat{\mathbf{n}}. \tag{58}$$

We could further proceed in this way in order to calculate the spin-polarizations after each subsequent collision. Actually, it is more helpful to make use of the recursive formula [see Eq. (25)]

$$\mathbf{P}_{m+1} = \frac{\mathbf{P}_m\cdot\hat{\mathbf{n}}+S(\vartheta)}{1+(\mathbf{P}_m\cdot\hat{\mathbf{n}})\,S(\vartheta)}\hat{\mathbf{n}}, \tag{59}$$

or

$$P_{m+1} = \frac{P_m+S(\vartheta)}{1+P_m\,S(\vartheta)}, \tag{60}$$

where

$$P_m = \mathbf{P}_m\cdot\hat{\mathbf{n}}, \tag{61}$$

with the initial condition $P_0 = 0$.

3.5. Full spin-polarization

It is quite easy to demonstrate that an initially unpolarized beam approaches full (transverse) spin-polarization after a number of elastic collisions occurring in the same plane of scattering and with identical scattering angles. This number depends on the target atom, the initial energy, and the scattering angle ϑ. Indeed, if

$$P_\infty \equiv \lim_{m\to\infty} P_m, \tag{62}$$

then we have

$$P_\infty = \frac{P_\infty+S(\vartheta)}{1+P_\infty\,S(\vartheta)}, \tag{63}$$

or, equivalently

$$\lim_{m\to\infty} P_m = \pm 1. \tag{64}$$

In Table 1 we have represented the change of spin-polarization (for an initially unpolarized beam) as a function of the number of elastic collisions. The first column represents the number of collisions, while the other columns refer to five different values of the Sherman function (0.1, 0.3, 0.5, 0.7, 0.9), i.e., the spin-polarization after the first collision (first row). The plane of scattering and the scattering angle are here assumed to be identical for all the sequences of elastic collisions. The values of the Sherman function depend on the chosen scattering angle. Full spin-polarization is reached after a number of collisions which depends on the value of Sherman function, i.e., on the selected scattering angle. The higher the Sherman function value, the smaller the number of elastic collisions necessary to reach full spin-polarization. From Table 1 we see that, selecting the scattering angle ϑ so that $S(\vartheta)$=0.5, after seven elastic collisions spin-polarization reaches 0.999. On the other hand, with $S(\vartheta)$=0.1, in order to reach 0.999 much many collisions are necessary. Note that, since we are considering here the special case in which all the collisions occur in the same scattering plane, the spin-polarization is always normal to it.

3.6. Conservation of spin-polarization for forward and backward elastic scattering

Note that the direct and spin-flip scattering amplitudes are given by [10]

$$f(\vartheta) = \frac{1}{2ik}\sum_{l=0}^{\infty}\{(l+1)\,[\exp(2i\eta_l^+)-1]+l\,[\exp(2i\eta_l^-)-1]\}P_l(\cos\vartheta), \tag{65}$$

$$g(\vartheta) = \frac{1}{2ik}\sum_{l=1}^{\infty}[-\exp(2i\eta_l^+)+\exp(2i\eta_l^-)]P_l^1(\cos\vartheta), \tag{66}$$

where k is the modulus of the electron momentum before scattering, η_l^+ and η_l^- are the phase shifts, $P_l(\cos\vartheta)$ the Legendre polynomials, and

$$P_l^1(x) = \sqrt{1-x^2}\,\frac{dP_l(x)}{dx}. \tag{67}$$

When $\vartheta = 0$ deg (forward elastic scattering) and when $\vartheta = 180$ deg (backward elastic scattering), $P_l^1(\cos\vartheta) = 0$, so that

$$g = 0 \tag{68}$$

regardless of the values of the phase shifts. As a consequence, for forward and backward elastic scattering, we have $S = 0$, $T = 1$, and $U = 0$. It follows from Eq. (25) that the final polarization does not change after forward or backward elastic scattering:

$$\mathbf{P}^f = (\mathbf{P}\cdot\hat{\mathbf{n}})\,\hat{\mathbf{n}} + \mathbf{P} - (\mathbf{P}\cdot\hat{\mathbf{n}})\,\hat{\mathbf{n}} = \mathbf{P}. \tag{69}$$

See, for example, Fig. 3. It was obtained assuming that the target atom was Xe, the electron energy was 900 eV, and, before scattering, the components of the spin-polarization were $P_x = 0.1$, $P_y = 0.2$, and $P_z = 0.3$, and the azimuthal angle was 60 deg. We can see, from Fig. 3, that the components of the spin-polarization do not change after forward and backward scattering. Actually, this result is general. Regardless of the target atom, the electron energy, the initial value of the spin-polarization, and the azimuthal angle, the spin-polarization for forward and backward elastic scattering is conserved.

4. Conclusions

We used density-matrix formalism to investigate spin-polarization phenomena in the electron–atom elastic scattering. We described the SPAS code, a computer program written to calculate the spin-polarization of an electron beam after scattering. We also treated the case of multiple scattering in order to study the evolution of the spin-polarization after several elastic collisions, demonstrating that an initially unpolarized beam becomes fully polarized in the direction normal to the scattering plane after a number of collisions occurring in

the same scattering plane and with identical scattering angles. Finally, we demonstrated that spin-polarization is conserved for forward and backward elastic scattering.

CRediT authorship contribution statement

Maurizio Dapor: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Resources, Data curation, Writing – original draft, Writing – review & editing, Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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