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Monte Carlo study of the effective Sherman function for electron polarimetry

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ABSTRACT

The PEBSI Monte Carlo simulation was upgraded towards usefulness for electron Mott polarimetry. The description of Mott scattering was improved and polarisation transfer in Møller scattering was included in the code. An improved agreement was achieved between the simulation and available experimental data for a 100 keV polarised electron beam scattering off gold foils of various thicknesses. The dependence of the effective Sherman function on scattering angle and target thickness, as well as the method of finding optimal conditions for Mott polarimetry measurements were analysed.

1. Introduction

The polarisation degree of freedom allows various important observables in atomic, molecular, nuclear, and particle physics to be accessed. It is, therefore, mandatory to provide accurate information about the degree of polarisation, both for an incident polarised particle beam and for a polarised particle produced in a reaction process. For the case of electrons at energies not exceeding about 10 MeV, Mott polarimetry[1] has been established as a standard tool (cf. [1] and references therein).

The method of electron Mott polarimetry is based on measuring azimuthal asymmetry (arising from the spin–orbit interaction) in scattering of a polarised electron beam off thin targets made of heavy elements. The differential cross section for Mott scattering on a single atom is given by the formula [2]:

$$\left(\frac{d\sigma}{d\Omega}\right)_{Mott} = \left(\frac{d\sigma}{d\Omega}\right)_0 \left(1 + S(E,\theta)\vec{P}\vec{n}\right), \quad (1)$$

where the cross section $(d\sigma/d\Omega)_0$ corresponds to scattering of unpolarised electrons, $S(E,\theta)$ is the Sherman function (i.e. the analysing strength of Mott scattering), E – kinetic energy of the beam and θ – polar scattering angle, $\vec{P}$ is the electron polarisation vector and $\vec{n}$ – the unit vector normal to the scattering plane: $\vec{n} = \vec{p} \times \vec{p}\,'/|\vec{p} \times \vec{p}\,'|$, where $\vec{p}$ and $\vec{p}\,'$ denote the momenta of the incoming and scattered electron, respectively.

The measurement can be performed using two counting detectors, denoted L and R, placed symmetrically about the beam axis, at a given angle θ. The asymmetry is then defined as: $A_{LR} = (N_L - N_R)/(N_L + N_R)$, where N_L and N_R are the number of counts observed in respective detectors for a given number of incident electrons; it is related to the component of the polarisation vector parallel to $\vec{n}$ as follows:

$$\vec{P}\vec{n} = A_{LR}/S. \quad (2)$$

The asymmetry reaches its maximum when the polarisation vector is perpendicular to the scattering plane.

The Sherman function, $S(E,\theta)$ in Eq. (1), strictly refers to scattering off a single atom; for a given material this function depends on the electron energy, E, and the scattering angle, θ. It can be calculated theoretically under assumptions regarding details of atomic and nuclear structure; the formalism was first given by Sherman [3]. In practice, the degree of polarisation is determined from asymmetry measured on targets of finite thicknesses, d. It is then appropriate in Eq. (2) to substitute the effective Sherman function

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[1] Throughout this paper we focus on electrons incident on thin Au foils only, although the method is also applicable to other targets and particles, e.g. protons.

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instead, $S_{\mathrm{eff}}(E,\theta,d)$. Multiple interactions of electrons with atoms[2] contribute to altering the electron direction of motion as well as orientation of its polarisation vector during passage through matter (resulting in beam depolarisation), which leads to a decrease of the effective Sherman function in targets of finite thicknesses w.r.t. that for a single atom.

These effects are too complex to be calculated analytically and simulation tools must be used for modelling the passage of polarised electrons through matter. Although the effective Sherman function can be measured and parametrised in terms of d, using data collected for targets of varying thicknesses, available measurements are scarce and cover only few energies. In view of the above, it is desirable to have a reliable tool which would allow to predict the effective Sherman function for arbitrary target thicknesses in yet unmeasured regions of kinematical variables. Meanwhile, precise simulation of these processes can be achieved within the PEBSI package [4] (**P**olarized **E**lectron **B**remsstrahlung **SI**mulator), which was originally developed to model target-thickness effects of bremsstrahlung emission from polarised electrons [5,6].

There were other Monte Carlo simulations written for similar purposes in the past (e.g. [7,8]); however, we do not know of any code including polarised electron scattering available to the public.[3] Furthermore, having very good models of relevant processes (electron-nucleus scattering, Møller scattering, electron impact ionisation) at our disposal encouraged us to use the most recent and hopefully the most appropriate treatment of these interactions.

A related problem which requires an a priori knowledge of the effective Sherman function is that of quantifying optimal conditions for measuring polarisation with the Mott polarimetry method for a given beam energy. The criterion, which balances sensitivity to polarisation vs. sample size, follows from considering the figure-of-merit, $\mathscr{F}$, defined as the product:

$$\mathscr{F}(E,\theta,d) \propto S_{\mathrm{eff}}^2(E,\theta,d)\,N(E,\theta,d), \tag{3}$$

where N is the total number of scattered electrons recorded in both counters. In this expression, S_{eff} is a decreasing and N is an increasing function of target thickness. Determining optimal conditions for a measurement resolves itself into choosing the values of target thickness and scattering angle that maximise the figure-of-merit. This issue is also addressed on the basis of our simulations below.

The aim of the present work was to improve the polarised electron transport treatment within the PEBSI code and to perform a thorough study of results regarding the simulated effective Sherman function, its parametrisation in terms of target thickness and measurement optimisation. Predictions for S_{eff} are compared to results obtained from measurements for 100 keV electrons scattering on several thin Au foils ($10 \div 500$ nm)[4] [11].

2. Upgrade of the PEBSI package

In the PEBSI package four basic processes of electron interaction with matter were explicitly considered: (*i*) Mott scattering (electron-nucleus); (*ii*) Møller scattering (electron scattering on quasi-free atomic electrons), (*iii*) electron impact ionisation (electron scattering on bound atomic electrons) and (*iv*) bremsstrahlung emission.[5]

The formalism of (*i*) was taken from the work of Kessler [12]; the ELSEPA package [13] – a numerical implementation of the formalism originally proposed by Sherman [3] – was used to calculate the scattering amplitudes, which determine the theoretical Sherman function and the change of the polarisation vector.

If the binding energy of the target electrons can be neglected (compared to the kinetic energy transferred to them in a collision) the electron–electron scattering process is described by the Møller cross section for scattering on free electrons. The approximation of a free target electron was applied to all electrons with binding energies $I_i < E_{\mathrm{thr}}$, where E_{thr} denotes the threshold energy to be set by the user of the code.

The contribution of Møller scattering to the effective Sherman function stems from the fact that any of the final state Møller electrons can be Mott-scattered into the detectors. However, momentum vectors of the Møller electrons are not aligned with the beam direction (w.r.t. which θ is measured), their energies as well as polarisations can be much different from those of the beam electrons. Counting these electrons leads to a decrease of the asymmetry value. Thus far polarisations of both outgoing Møller electrons were neglected (set to zero) in PEBSI. This turns out to be a good approximation for the lower energy secondary electron but inadequate for the higher energy one (scattered at a small angle). This is illustrated in Fig. 1. In the symmetric scattering configuration ($\theta = 43.7^\circ$ for a 100 keV incident electron) both outgoing electrons have the same polarisation; however, in an asymmetric configuration, in particular for very small scattering angles, the electron with higher energy inherits most of the incoming electron polarisation. Therefore we have supplemented PEBSI with a code describing polarisation of outgoing Møller electrons.

The polarisation state of these electrons is described by a density matrix, ρ_{out} [14]. Since the secondary electrons can be entangled, they do not have, in general, a well determined polarisation state. Nevertheless, one can assign mean polarisation vectors to both of them. In order to calculate the mean polarisation vector of the ith secondary electron, a partial trace operation over the other one, jth, was performed, yielding a reduced density matrix: $\rho_i = \mathrm{Tr}_j \rho_{out}$. Next, the mean polarisation vector for the ith electron, $\vec{P}_i$, was calculated as: $\vec{P}_i = \mathrm{Tr}(\rho_i \cdot \boldsymbol{\sigma})$, where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ and σ_k are the Pauli matrices.

The model of Møller scattering is valid only in case of scattering of free particles. In case of scattering off bound electrons both the cross section and the energy distribution are different, as the binding energy has to be taken into account. Therefore, for target electron shells with binding energies $I_i \geqslant E_{\mathrm{thr}}$ the (total) electron impact ionisation cross sections provided by the formula proposed by Bote et al. [15] were used. These cross sections result from an algorithm that approximates a database generated by rigorous PWBA and DWBA calculations.[6] The MRBEB[7] model recently developed by Guerra et al. [16] was used to obtain also the energy differential cross sections (since the approach of Bote et al. yields only the total cross sections).

The polarisation of the outgoing electrons is obtained applying the treatment for Møller scattering. We expect this method to yield reasonable results as long as $\Delta E \gg I_i$, i.e. when the binding of the target electron is of minor importance to accurately describe the collision (much smaller than the energy loss ΔE).

Apart from the new implementation of Møller scattering, the description of Mott scattering was improved and several shortcomings corrected, resulting in an improved agreement of the simulation results with the data.

[2] The mean free path length between two subsequent interactions is typically smaller than feasible target thicknesses, cf. footnote 4.

[3] We have not encountered a satisfactory description of Mott scattering in the commonly used Geant4 package [9] or the EGS5 code [10].

[4] For 100 keV electrons scattering off a gold target the mean free path length between two elastic electron-atom collisions is about 8 nm.

[5] In the discussed case emission of a bremsstrahlung photon accompanied by a significant change in electron polarisation has a very small cross section compared to other considered interactions; therefore it was neglected in the present work.

[6] Plane-wave and distorted-wave Born approximations.

[7] Modified Relativistic Binary Encounter Bethe model.