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Monte Carlo calculation of large and small-angle electron scattering in air

B.I. Cohen *, D.P. Higginson, C.D. Eng, W.A. Farmer, A. Friedman, D.P. Grote, D.J. Larson

Lawrence Livermore National Laboratory P. O. Box 808 Livermore, CA 94551, United States

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ABSTRACT

A Monte Carlo method for angle scattering of electrons in air that accommodates the small-angle multiple scattering and larger-angle single scattering limits is introduced. The algorithm is designed for use in a particle-in-cell simulation of electron transport and electromagnetic wave effects in air. The method is illustrated in example calculations.

1. Introduction

The scattering of electrons in foils or air has received considerable attention over many years in publications addressing theory, experiment, and simulation. Here we report the introduction of a new algorithm for constructing and Monte Carlo sampling a probability distribution function (PDF) for the scattering angle of an electron colliding with atoms. The PDF is a composite distribution capturing the Gaussian distribution of multiple small-angle scatters and the non-Gaussian, Rutherford tail at larger angles. We propose an algorithm extending existing theory and illustrate its use in example calculations. The algorithm is implemented in a Monte Carlo particle-in-cell code. In a companion paper [1], Higginson introduces the approach to building a composite PDF by solving the set of constraint equations used here. However, Higginson's solution method and implementation in a code are quite different: the solution for the composite PDF is done in the loop over particles when the scattering is performed. Moreover, Higginson extends the PDF to large scattering angles, verifies his methodology with comparisons against direct Monte Carlo scattering computations using the Rutherford cross-section, and applies his new hybrid method to entirely different physics applications.

The introduction of a new algorithm and the demonstration of its use herein are motivated by the goal of including both large-angle and multiple small-angle elastic collisions in a Monte Carlo treatment of elastic and inelastic scattering of electrons within an electromagnetic particle-in-cell (PIC) simulation code designed for use in various physical applications. The development of the model for the algorithm demonstrates the simplicity of the approach, and the example calculations give some insight into the relative accuracy of the model when compared to experimental data and other theories on angle scattering of electrons and the limits on precision due to statistical resolution in the Monte Carlo simulations.

* Corresponding author.
E-mail address: cohen1@llnl.gov (B.I. Cohen).

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2. Formulation

The theory of electron scattering is well established [2–8]. Here we follow the treatment by Jackson in Secs. 13.6 and 13.7 of his classic textbook [6]. We are not aware that Jackson's treatment of large and small angle scattering has been used previously as the basis for a Monte Carlo treatment of electron scattering by neutral matter. For electron energies in excess of 1 keV of interest in our applications, the mean-square-deflection angle (polar angle relative to the incident velocity of the electron) for a single scatter is given by

$$\langle\theta^2\rangle \approx 2\theta_{min}^2 \ln\left(\frac{\theta_{max}}{\theta_{min}}\right) \to 2\theta_{min}^2 \ln\left(\frac{192}{Z^{1/3}}\frac{p}{m_e c}\right) \tag{1}$$

where $\theta_{max} = 1$ and $\theta_{min} = (Z^{1/3}/192)(m_e c/p)$ in this limit, p is the electron momentum, and Z is the atomic number of the medium in which the electrons are scattered. The numerical factor 192 in Eq. (1) arises from the ratio of the atomic radius $a \approx 1.4a_0 Z^{-1/3}$ to the electron Compton wavelength, where a_0 is the hydrogenic Bohr radius, and the use of the definition of the fine-structure constant. In this treatment of the electron experiencing the rare larger angle event, the scattering angle is large compared to the root-mean-square angle but is still small, < 1, in an absolute sense. The approximation that one can set $\theta_{max} = 1$ introduces some imprecision through the term $\ln(\theta_{max}/\theta_{min})$, which is common in Coulomb collision theory.

Jackson shows that the mean-square angular deflection $\langle\Theta^2\rangle$ after an electron beam traverses a thickness $d = v\Delta t$ is given by

$$\langle\Theta^2\rangle \approx 2\pi n_a v\Delta t\left(\frac{2Ze^2}{pv}\right)^2 \ln\left(\frac{1}{\theta_{min}}\right) \to 2\frac{Z\omega_{pe}^2 r_e}{c}\frac{m_e^2 c^2}{p^2}\frac{c}{v}L_s\Delta t \tag{2}$$

$$L_s = \ln\left(\frac{1}{\theta_{min}}\right) = \ln\left(\frac{192}{Z^{1/3}}\frac{p}{m_e c}\right) \tag{3}$$

where v is the electron speed, Δt is the time step, n_a is the atomic number density of the scattering medium, ω_{pe} is the electron plasma frequency with $\omega_{pe}^2 = 4\pi n_a Ze^2/m_e$, and $r_e = e^2/m_e c^2$ is the classical electron radius. The number of collisions experienced by an electron in the thickness d is given in Jackson's Eq. (13.109):

$$N_{coll} = n_a\sigma d \approx \pi n_a v\Delta t\left(\frac{2Ze^2}{pv}\right)^2 \frac{1}{\theta_{min}^2} = 4\pi n_a v\Delta t\left(192 Z^{2/3}\frac{c}{v}\frac{e^2}{m_e c^2}\right)^2 \tag{4}$$

The thickness d must be sufficiently large so that $N_{coll} >> 1$ but not so large that inelastic collisions change the electron energy appreciably nor allow the electron to transport in space far enough for the scattering medium to have changed significantly. The latter constraint serves to justify adopting an operator-splitting approach in incorporating Monte Carlo angle scattering as well as an inelastic collision model within an electromagnetic PIC simulation.

Jackson finds it convenient to transform coordinates from spherical polar coordinates aligned with the incident electron momentum vector to coordinates where θ is projected onto a fixed plane in the laboratory frame $(\theta, \phi) \to (\theta', \phi')$ (Fig. 13.7 of Ref. [6]) such that $\langle\theta'^2\rangle \approx \langle\frac{1}{2}\theta^2\rangle$. The small-angle electron Rutherford differential cross-section per atom becomes

$$\frac{d\sigma}{d\Omega}(\theta,\phi) \approx (\frac{2Ze^2}{pv})^2\frac{1}{\theta^4} \to \frac{d\sigma}{d\Omega}(\theta',\phi') \approx (\frac{2Ze^2}{pv})^2\frac{1}{4\theta'^4} \tag{5}$$

Jackson then integrates the differential cross-section $(d\sigma/d\Omega)sin\theta' d\theta' d\phi' \approx (d\sigma/d\Omega)\theta' d\theta' d\phi'$ with respect to ϕ' to obtain the reduced differential cross-section

$$\frac{d\sigma}{d\theta'}(\theta') = \oint \frac{d\sigma}{d\Omega}(\theta',\phi')d\theta' d\phi' \approx \frac{\pi}{2}(\frac{2Ze^2}{pv})^2\frac{1}{\theta'^3} \tag{6}$$

and the single-scattering distribution for the projected angle is then

$$P_S(\theta')d\theta' = n_a v\Delta t\frac{d\sigma}{d\theta'}(\theta')d\theta' \approx \frac{\pi}{2}n_a v\Delta t(\frac{2Ze^2}{pv})^2\frac{d\theta'}{\theta'^3} \tag{7}$$

which is Jackson's Eq. (13.114) if we recall $d = v\Delta t$. At this point Jackson scales the scattering angle θ' in terms of the root-mean-square scattering angle $\langle\Theta^2\rangle^{1/2}$, i.e., $\alpha \equiv \theta'/\langle\Theta^2\rangle^{1/2} = \theta/\langle 2\Theta^2\rangle^{1/2}$. The single-scattering distribution is valid for angles that are large compared to $\langle\Theta^2\rangle^{1/2}$. The distribution for multiple small-angle scattering tends to a Gaussian as dictated by the central limit theorem. Restricting the polar scattering angle to be positive leads to the following expressions for the multiple and single-scattering distributions and the composite distribution P:

$$P(\alpha)d\alpha = P_M(\alpha)d\alpha = \frac{2c_{norm}}{\sqrt{\pi}}e^{-\beta\alpha^2}d\alpha, \alpha < \alpha_t \tag{8}$$

$$P(\alpha)d\alpha = P_S(\alpha)d\alpha = \frac{1}{2L_s}\frac{d\alpha}{\alpha^3}, \alpha \geq \alpha_t \tag{9}$$