

Correlation between multiple scattering angle and ionization energy loss for fast electrons. Prospects for experimental observation

M.V. Bondarenco

NSC Kharkov Institute of Physics & Technology, Kharkov, Ukraine
V. N. Karazin Kharkov National University, Kharkov, Ukraine

June 11, 2025, French-Ukrainian Workshop, IJCLab, Paris-Saclay University, France

- 1 Introduction
- 2 Solution of the transport equation
- 3 Computed distributions
- 4 Angular dependence of the mean energy loss
- 5 Summary

Introduction. I

Molière [1] and Landau [2] theories describe correspondingly multiple Coulomb scattering and ionization energy loss by fast charged particles in matter, but **leave the question whether there is a correlation between those processes unanswered.**

For a high-energy charged particle, the dominant contribution to correlation between its energy loss and deflection angle arises when the fast particle **hits an atomic electron**, imparting it energy and transverse momentum simultaneously.

The correlation must be the strongest when the **incident particle is an electron or positron**, because having the same mass as the knocked-off atomic electrons, it is kinematically allowed to transfer them a substantial fraction of its energy in a single collision.

Introduction. II

In a thick target, the angle-energy correlation generally **disappears** due to successive interactions with **many** atoms.

But in multiple Coulomb scattering of **pointlike** particles there is a significant contribution from **single scatterings**, purporting the **correlation**.

The correlation is expected to be stronger for **low- Z target materials**, because the relative contribution of incoherent scattering for them is higher.

Vanishing of the correlation for normal multiple scattering. I

After N successive identical random collisions, with individual χ_k^2 and $\Delta\epsilon_k$ correlated for the same k , the correlation coefficient between the aggregate energy loss $\epsilon = \sum_{k=1}^N \Delta\epsilon_k$ and the square of the deflection angle $\vec{\theta} = \sum_{k=1}^N \vec{\chi}_k$ is defined as

$$C = \frac{\langle (\theta^2 - \langle \theta^2 \rangle)(\epsilon - \langle \epsilon \rangle) \rangle}{\sqrt{\langle (\theta^2 - \langle \theta^2 \rangle)^2 \rangle} \sqrt{\langle (\epsilon - \langle \epsilon \rangle)^2 \rangle}}. \quad (1)$$

If **all** the single-scattering **mean values are finite** (multiple scattering is normal), evaluation of (1) gives

$$C = \frac{\langle \chi^2 \Delta\epsilon \rangle - \langle \chi^2 \rangle \langle \Delta\epsilon \rangle}{\sqrt{\langle \chi^4 \rangle + (N-2)\langle \chi^2 \rangle^2} \sqrt{\langle (\Delta\epsilon - \langle \Delta\epsilon \rangle)^2 \rangle}} \stackrel{N \gg 1}{\sim} \frac{1}{\sqrt{N}} \rightarrow 0, \quad (2)$$

implying that in the large- N limit (multiple scattering) the correlation must vanish.

Vanishing of the correlation for normal multiple scattering. II

The joint distribution function then tends to a product of a Gaussian and a delta function

$$f(\vec{\theta}, \epsilon, l) \xrightarrow{N \rightarrow \infty} \frac{1}{\pi \langle \theta^2 \rangle} e^{-\theta^2 / \langle \theta^2 \rangle} \delta(\epsilon - \langle \epsilon \rangle).$$

Here the mean values are in proportion $\langle \theta^2 \rangle / \langle \epsilon \rangle = \langle \chi^2 \rangle / \langle \Delta \epsilon \rangle$, but no correlation arises between θ and ϵ . In the presented derivation it was essential that $\langle \epsilon \rangle \sim N \gg \sqrt{\langle (\epsilon - \langle \epsilon \rangle)^2 \rangle} \sim \sqrt{N}$, whereas for θ the same does not hold, because $\langle \vec{\theta} \rangle = N \langle \vec{\chi} \rangle = 0$ by axial symmetry.

But for multiple **Coulomb** scattering the diffusion is **not** normal ($\langle \chi^2 \rangle = \infty$).

Transport equation. I

The correlated process of small-angle scattering of a fast electron on atoms in an amorphous substance, and of the associated ionization energy loss, is governed by a transport equation

$$\begin{aligned} \frac{\partial}{\partial l} f(\vec{\theta}, \epsilon, l) = & -n_a \int d\sigma_{el}(\chi) \left[f(\vec{\theta}, \epsilon, l) - f(\vec{\theta} - \vec{\chi}, \epsilon, l) \right] \\ & - n_a \iint d\sigma_{in}(\chi, \Delta\epsilon) \left[f(\vec{\theta}, \epsilon, l) - f(\vec{\theta} - \vec{\chi}, \epsilon - \Delta\epsilon, l) \right], \end{aligned} \quad (3)$$

which must be subjected to initial condition $f(\vec{\theta}, \epsilon, 0) = \delta(\vec{\theta})\delta(\epsilon)$.
The anomalous character of multiple inelastic Coulomb scattering enters through the Rutherford asymptotics of the elastic scattering

$$n_a l d\sigma_{el}(\chi) \underset{\chi \gg \chi_a}{\simeq} n_a l d\sigma_{Ruth}(\chi) = 2Z^2 \bar{\chi}_c^2 \frac{d\chi}{\chi^3}, \quad (4)$$

and inelastic scattering differential cross-sections:

$$n_a l d\sigma_{in}(\chi, \Delta\epsilon) \underset{\chi \gg \chi_a}{\simeq} 2Z \bar{\chi}_c^2 \delta\left(\Delta\epsilon - \frac{p^2}{2m} \chi^2\right) \frac{d\chi}{\chi^3} d\Delta\epsilon. \quad (5)$$

Transport equation. II

Here $\frac{d\sigma_{Ruth}}{d\chi} = \frac{8\pi Z^2 e^4}{p^2 v^2 \chi^3}$, with Ze the atom nucleus charge, and v the particle velocity, p its momentum.

The factor [3]

$$\bar{\chi}_c^2 = \frac{4\pi e^4 n_a l}{p^2 v^2} \quad (6)$$

incorporates all the properties of the target except Z .

Correlated solution in the multiple scattering regime. I

The resulting distribution function depends on the following dimensionless variables:

$$\Theta = \theta / Z \bar{\chi}_c, \quad (\text{reduced deflection angle}) \quad (7)$$

$$\lambda(Z, l, \epsilon) = \frac{2m}{p^2 Z \bar{\chi}_c^2} \epsilon - \lambda_0, \quad \lambda_0 = \ln \frac{p^2 \gamma^2 Z \bar{\chi}_c^2}{l_\delta'^2} - \gamma_E + \gamma^{-2}, \quad (8)$$

with l – the mean ionization potential,

$$y_0(l, Z) = 4Z \left(Z \bar{\chi}_c^2 / \chi_{at}'^2 \right)^{1+1/Z} e^{\gamma_E/Z} \gg 1 \quad (\text{thickness parameter}), \quad (9)$$

$$\chi_{at}' = \chi_a'^{\frac{Z}{Z+1}} \chi_{in}'^{\frac{1}{Z+1}} \quad (\text{screening angle}). \quad (10)$$

Correlated solution in the multiple scattering regime. II

The solution of the transport equation (3) is given by a double integral

$$\begin{aligned} \frac{p^2}{2m} Z^3 \bar{\chi}_c^4 f(Z, l, \theta, \epsilon) &= F(Z, y_0, \Theta, \lambda) \\ &= \frac{1}{4\pi} \int_0^{y_{\max}} dy J_0(\sqrt{y}\Theta) e^{\Omega_{el}(y_0, y)} \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} du e^{\lambda u + \Omega_{in}(y/4Z, u)}, \quad (11) \end{aligned}$$

with J_0 the Bessel function,

$$\Omega_{el}(y_0, y) = -\frac{y}{4} \ln \frac{y_0}{y} \quad (\text{the function appearing in the Molière theory}), \quad (12)$$

$$\Omega_{in}(Y, u) = (u + Y) [\ln u + \text{Ein}(Y/u)] + u (1 - e^{-Y/u}). \quad (13)$$

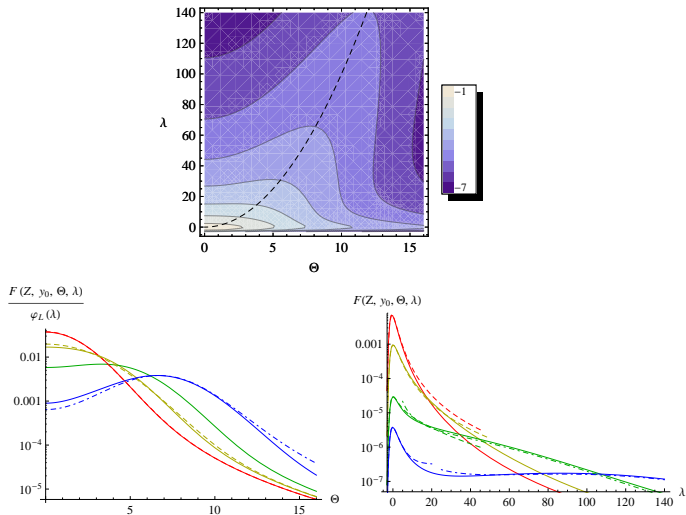


Figure 1: Correlated angle-energy loss distribution of electrons multiple scattered in hydrogen ($Z = 1$) target of reduced thickness $y_0 = 10^4$. a). Contour plot of $\log F$, with F given by Eq. (11). Dashed parabola, $\lambda = Z\Theta^2$. b). Angular distributions at fixed values of the ionization energy loss straggling variable λ . Solid curves, calculation by exact formula (11), at $\lambda = 0$ (red), $\lambda = 7$ (yellow), $\lambda = 20$ (green), $\lambda = 50$ (blue). c). Ionization energy loss distribution at fixed values of the scattering angle. Solid curve, $\Theta = 0$ (red), $\Theta = 4$ (yellow), $\Theta = 8$ (green), $\Theta = 16$ (blue).

$$\frac{F(Z, y_0, \Theta, \lambda)}{\varphi_L(\lambda)}$$

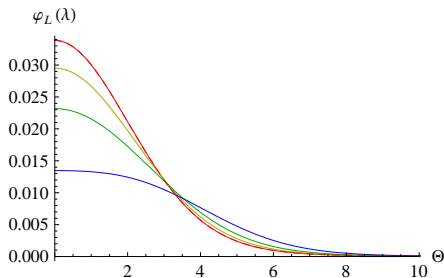


Figure 2: Angular distributions of electrons multiple scattered in a carbon ($Z = 6$) target of reduced thickness $y_0 = 10^4$, at fixed values of the ionization energy loss straggling variable λ : $\lambda = 0$ (red), $\lambda = 7$ (yellow), $\lambda = 20$ (green), $\lambda = 50$ (blue).

$$\frac{F(Z, y_0, \Theta, \lambda)}{\varphi_L(\lambda)}$$

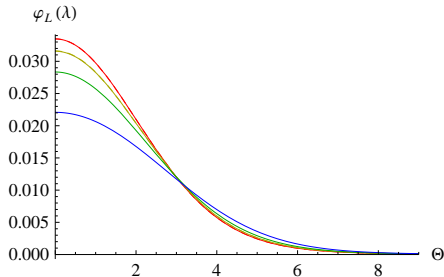


Figure 3: The same as Fig. 2, for silicon ($Z = 14$) target of reduced thickness $y_0 = 10^4$.

Normalized correlation function

The magnitude of the correlation may be quantified by introducing the normalized correlation function

$$g(Z, y_0, \Theta, \lambda) = \frac{Z+1}{Z} \frac{F(Z, y_0, \Theta, \lambda)}{\varphi_L(\lambda) \varphi_M \left(\frac{4\chi_c^2}{\chi_{at}^2}, \frac{\theta}{\chi_c} \right)}. \quad (14)$$

Here in the denominator

$$\begin{aligned} 2\pi \int_0^\infty d\Theta \Theta F(Z, y_0, \Theta, \lambda) &= \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} du e^{\lambda u + \Omega_{in}(0, u)} \\ &= \varphi_L(\lambda) \end{aligned}$$

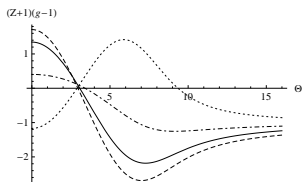
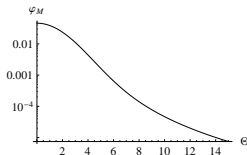
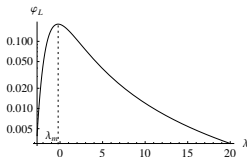
is the Landau distribution, and

$$\int_{-\infty}^\infty d\lambda F(Z, y_0, \Theta, \lambda) = \frac{Z}{Z+1} \varphi_M \left(\frac{4\chi_c^2}{\chi_{at}^2}, \frac{\theta}{\chi_c} \right),$$

with $\chi_c^2 = Z(Z+1)\bar{\chi}_c^2$,

$$\varphi_M(\eta_0, \Psi) = \frac{1}{4\pi} \int_0^{\eta_{\max}} d\eta J_0(\sqrt{\eta}\Psi) e^{-\frac{\eta}{4} \ln \frac{\eta_0}{\eta}}, \quad (15)$$

is the Molière distribution.



Angular dependence of the mean energy loss

An alternative possibility to express the correlation is to evaluate the conditional (fixed-angle) **mean** energy loss:

$$\bar{\epsilon}(\theta) = \frac{\int_0^\infty d\epsilon \epsilon f(\theta, \epsilon)}{\int_0^\infty d\epsilon f(\theta, \epsilon)} = \frac{p^2 Z \bar{\chi}_c^2}{2m} [\lambda_0 + \bar{\lambda}(\Theta)], \quad (16)$$

with

$$\bar{\lambda}(\Theta) = \frac{\int_{-\infty}^\infty d\lambda \lambda F(Z, y_0, \Theta, \lambda)}{\int_{-\infty}^\infty d\lambda F(Z, y_0, \Theta, \lambda)}, \quad (17)$$

$$\bar{\lambda}(Z, \eta_0, \theta/\chi_c) = \frac{2 \int_{\theta/\chi_c}^\infty d\psi \psi \varphi_M(\eta_0, \psi)}{\varphi_M(\eta_0, \theta/\chi_c)} - \ln \frac{\eta_0}{4(Z+1)} - \gamma_E, \quad \eta_0 = \frac{4\chi_c^2}{\chi_{at}^2}. \quad (18)$$

It expresses, in the integral form, solely through the Molière distribution φ_M .

$\bar{\lambda}(Z, \eta_0, \theta/\chi_c) - \ln(Z+1)$

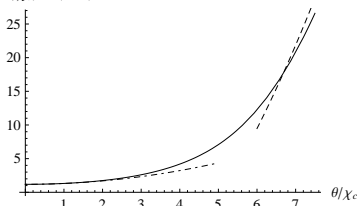


Figure 4: Solid curve, dependence of the mean energy loss defined by Eq. (18) on the scattering angle, for a reduced target thickness $\eta_0 = 10^4$.

Summary

- The amalgamation of Molière and Landau theories reveals a substantial correlation between the deflection angle and ionization energy loss for relativistic electrons in amorphous matter. The correlation arises at the single-scattering level, but is not erased by multiple Coulomb scattering, because of the anomalous character of the latter.
- The domain of applicability of the combined theory is just the intersection of the domains of applicability of Molière and Landau theories.
- The experimental verification of the expected correlation must be feasible with silicon targets (the lowest- Z industrial semiconductor), by looking for $\sim Z^{-1} \approx 10\%$ differences between the angular distributions measured at different values of the ionization energy loss.
Stronger correlation effects ($\sim Z^{-1} \approx 20\%$) are expected for organic semiconductors, used nowadays for flexible electronics [7].

References



G. Molière,
Z. Naturforsch. **3a**, 78 (1948).



L. D. Landau,
J. Phys. (Moscow) **8**, 201 (1944).



U. Fano,
Phys. Rev. **93** (1954) 117.



J. F. Bak *et al.*,
NP B **288**, 681 (1987).



K. K. Andersen *et al.*,
NIM B **268**, 1412 (2010).



Y. Wang *et al.*,
Chem. Soc. Rev. **48**, 1492 (2019).



M. V. Bondarenco,
Phys. Rev. D **103**, 096026 (2021).