MOLIÈRE MODEL

- **Not really a *model* – more a difficult calculation**
  - **Little (if any) disagreement by the experts**
  - ***No free parameters***

- **All theories (models) fundamentally the same**

- **Nevertheless, MICE should compare measurements to a model**
  - ***Expect most – if any – discrepancy with LH2***
    - **Followed by LiH**

- **Molière has little to do with original PDG expression**
  - **Originated from Rossi & Griesen**

MICE COMPARISON

- **Data should – *must* – be compared with *direct* calculation of Molière distribution**

- **Some MC may be necessary**
  - **To allow for efficiencies, ‘no-absorber’, and acceptance**

  - **But don’t believe that what (say) G4 gives is pure Molière (or anything else) without very careful check**

  - **G4 et al have to be pragmatic and take various short cuts**
    - **Results may be good enough for most purposes, however**
    - ***Caveat emptor!***

OVERVIEW

- The underlying physics
  - Single scattering
- The ‘problem’
  - How to obtain the distribution of scattering angles
- What Molière did
  - But not in detail
- The recipe
  - But not in detail

- Comparison with another model

- Comments & To Do list

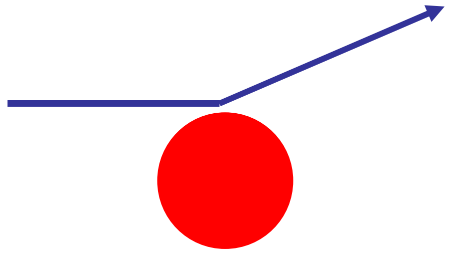
CRIBS USED IN FOLLOWING

- **Rossi's book 'High Energy Particles' circa 1956**

- **G. Molière, Z. Naturforsch, 3a, 78 (1948) (in German)**
- **H.A. Bethe, Phys. Rev. 89, No. 6, 1256 (1953) (in English)**
- **U. Fano, Phys. Rev. 93, No. 1, 117 (1954)**

- ***B. Gottschalk et al., NIM B74 467 (1993)***

UNDERLYING PHYSICS:
SINGLE SCATTERING



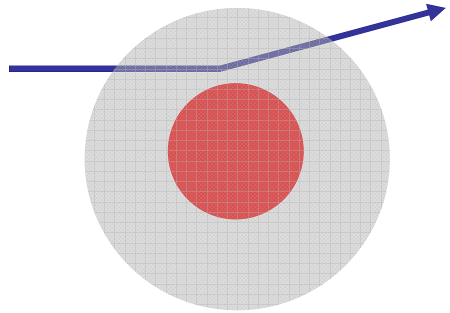
<u>Rutherford:</u>

Particle scatters from bare nucleus

Classical E-M

Coherent:

Z^2

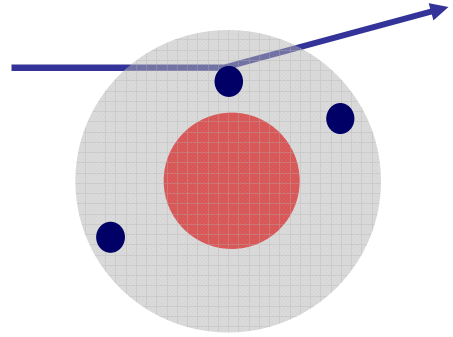


<u>Wentzl / Molière:</u>

Nucleus screened by atomic electrons

QM calculation

➔ Screening angle



Particle scatters from *atomic electrons themselves* – part of energy loss

Incoherent:

Z

Apart from atomic constants, *single scattering* cross-section from screened nucleus is:

$$\frac{d\sigma}{d\Omega} \propto \frac{Z^2}{pv} \frac{1}{(\chi_a^2 + \chi^2)^2}$$

$\frac{1}{pv}$ **is pure kinematics**

$$\chi_a = \frac{\hbar}{pa} = \frac{\lambda\!\!\!^{-}}{a} = \frac{\lambda\!\!\!^{-}}{0.885 a_o Z^{-\frac{1}{3}}}$$

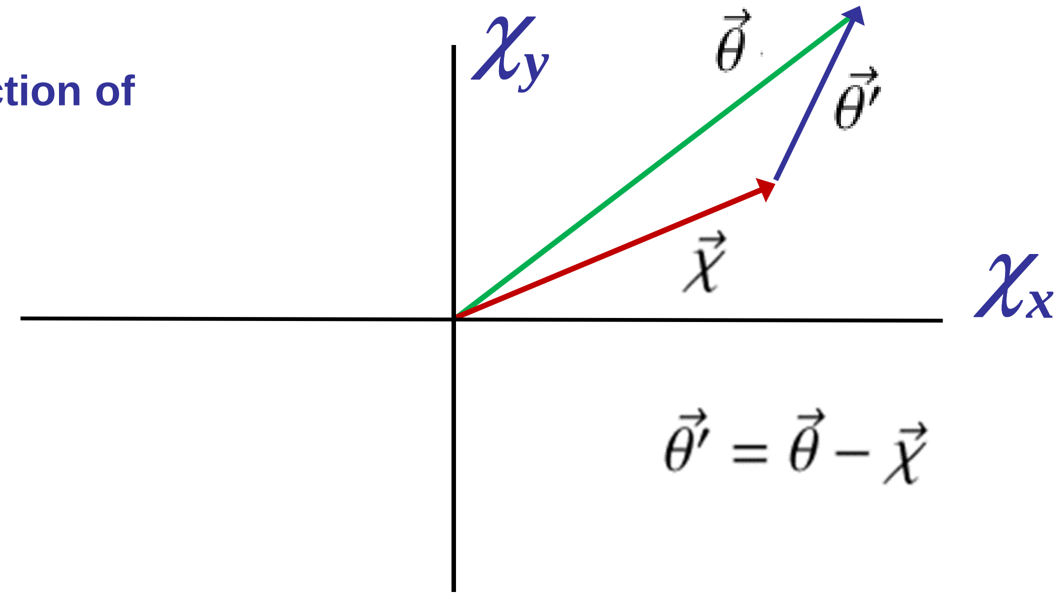
is screening angle, depending on *Z* but order of microradians

a **is Thomas-Fermi radius of atom**

***Ignores the atomic electrons* – but cross-section per atom smaller by *Z* – unimportant in medium or high-*Z* materials**

MULTIPLE SCATTERING

View in angular plane perpendicular to direction of incident particle



- ***The problem*** **is to determine the distribution of scattering angle after many (thousands) of single scatters**
- **Space angle is** θ
- ***Two dimensional*** **convolution;** χ **is a 2D** ***vector***

SOLVE TRANSPORT EQUATION:

Scattered out **Scattered in**

$$\frac{\partial f(\theta, t)}{\partial t} = -Nf(\theta, t)\int \sigma(\chi)\chi d\chi + N\int f(\vec{\theta}', t)\sigma(\chi)d\chi$$

$$\vec{\theta}' = \vec{\theta} - \vec{\chi}$$

$f(\theta, t)$ **is (desired) distribution of** θ **after thickness** t

N **is number density of scatterers**

Solve with Fourier – Bessel transformations (higher maths!)

MOLIÈRE

- **Used WKB method + T- F potentials to obtain** χ_a
- **Solved the transport equation**
- **Introduced** χ_c **, the 'single scattering angle'**
  - **Probability of scatter with** $\theta > \chi_c = 1$ **in thickness** t
- **Distribution** $f(\theta, t)$ **described by ratio** $\frac{\chi_c}{\chi_a}$ **and** χ_c **in terms of a scaled angle:**

In terms of a new parameter B :

$$B\left(\frac{\chi_c}{\chi_a}\right)$$

Molière angle :

$$2\theta_M^2 = \chi_c^2 B$$

Scaled angle :

$$\theta' = \frac{\theta}{\sqrt{2}\theta_M}$$

Final distribution of space angles :

$$f(\theta) = \frac{1}{2\pi\theta_M^2}\frac{1}{2}\left[f^{(0)}(\theta') + \frac{f^{(1)}(\theta')}{B} + \frac{f^{(2)}(\theta')}{B^2}\right]$$

THE FUNCTIONS

$$f^{(n)}(\theta') = \frac{1}{n!}\int_0^\infty y\,\mathrm{d}y J_0(\theta' y)\,\mathrm{e}^{-y^2/4}\left(\frac{y^2}{4}\ln\frac{y^2}{4}\right)^n . \tag{16a}$$

$f^{(0)}$ is simply a Gaussian:

$$f^{(0)}(\theta') = 2\,\mathrm{e}^{-\theta'^2}. \tag{16b}$$

Molière and Bethe give further formulas and tables for $f^{(1)}$ and $f^{(2)}$.

- **From Gottschalk's paper**

- **The *f*s are tabulated by Molière and Bethe (phew!)**
  - **at discrete values of θ'**

Tab. 2. Die Funktionen $f^{(1)}(\vartheta)$, $f^{(2)}(\vartheta)$, $f^{(1)}(\varphi)$ und $f^{(2)}(\varphi)$.

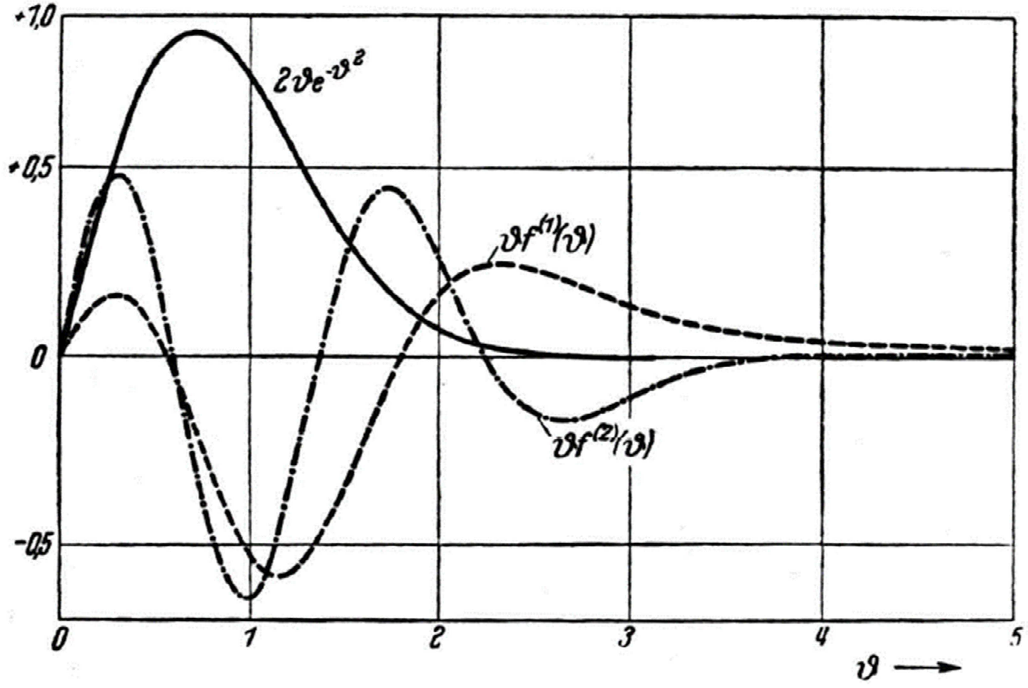


Abb. 1. Die Entwicklungskoeffizienten in Gl. (7, 3 a) für die Verteilung der räumlichen Streuwinkel.

Functions f^0, f^1 and f^2 from Molière's paper

BUT WHAT ABOUT THE ELECTRONS?

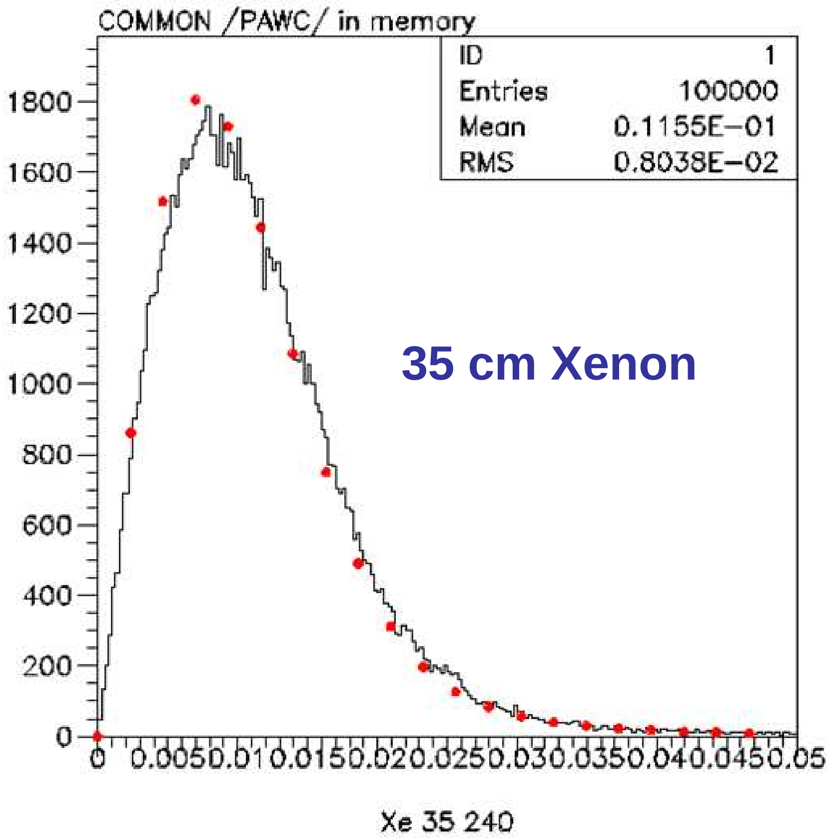
- **Bethe, following Kultchitsky and Latyshev, used the *ansatz***
  - $Z^2 \rightarrow Z(Z+1)$ **in expression for** χ_c
- **But does not allow for very different kinematics of scattering from nuclei or electrons**
  - **Maximum angle for 200 MeV/*c* muon from electron ~ 5 mr**
  - **~ 1 radian from nucleus**
- **Fano introduced better correction taking into account binding of electrons *and kinematics***
  - **Not easy to follow in detail**
  - **Used in Gottschalk's paper (and what follows)**

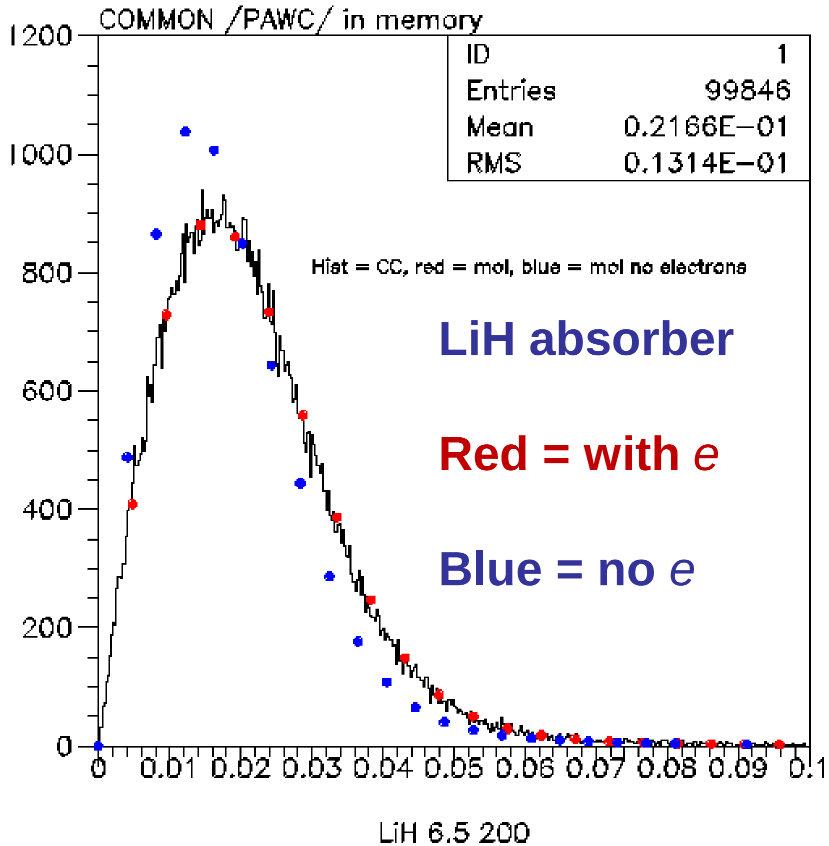
CALCULATIONS

- **Best 'recipe' is in Gottschalk's paper**
  - **Not difficult if you keep a clear head**
  - **Shows how, following Molière, to deal with:**
    - **Mixtures & compounds**
    - **Energy loss**
    - **Electrons**
      - **à la Fano**

  - **Tables for *space* (3D) *angle* from Bethe**
  - **Tables for *projected angles* (2D) from Molière**
    - **Both given only at a discrete set of θ_M up ~ 7 (4 in 2D)**
      - **Either interpolate or dreadful integral at each θ**

COMPARE C & C – MOLIÈRE





C & C is brute-force Monte Carlo of individual scatters, including electrons

Molière calculation follows Gottschalk's prescription, Bethe's tables

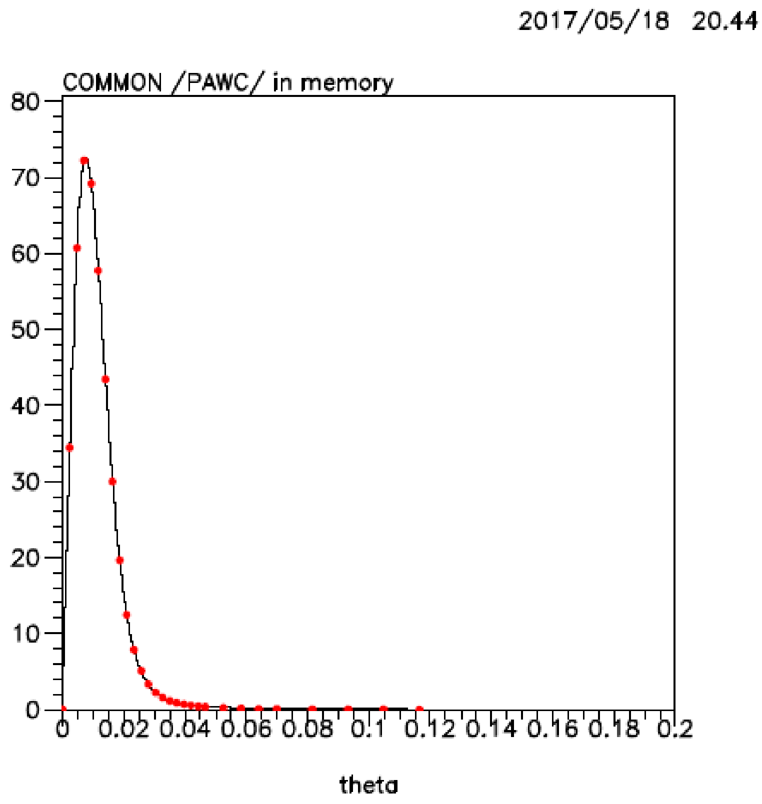
Looks good (as it should); electrons matter in LiH

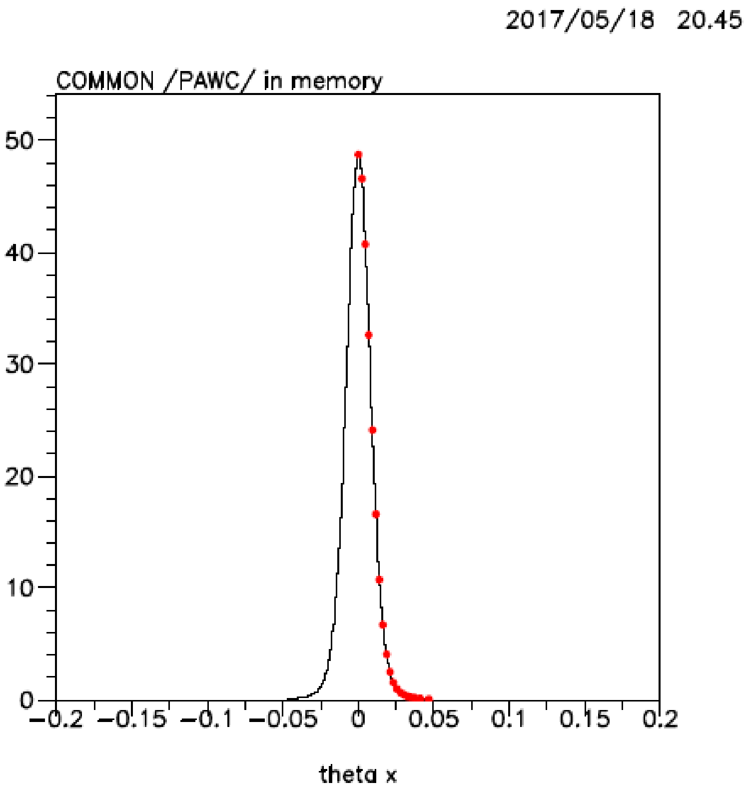
STATUS

- Have FTN (!) code that can
  - Calculate Molière distributions at discrete points
    - (as given by Molière and Bethe)
  - In 3D (space angle)
  - In 2D (projected angle)
  - Computation time is ‘zero’

  - Interpolate between points in 3D or 2D
    - Cubic spline

  - For LH2, LiH, Ne, Al, Xe, Scintillator…..
    - Easy to add others
  - Calculated for all MICE absorbers & momenta
    - → John N.





Example 3D and projected angle distributions (LiH, 240 MeV/c ???)

Points & interpolation

PLANS

- Range of angles given by Molière & Bethe is (a bit) limited
  - Extend range
    - Molière gives approximate formulas for larger angles
      - Claims are good to 2 – 3 percent

- Compare with Muscatt data
  - Including Fano correction
  - (don’t think Muscatt did that)

- Figure out convenient way of integrating over wide beam-momentum distributions

- Think about range of validity of convolution and de-convolution used in the analysis (data = pure absorber * no absorber)

IS MOLIÈRE CORRECT?

We have reviewed six other published proton measurements, partially reanalyzing four whose authors claimed that Molière theory either did not apply (because of thick targets) or was incorrect. These experiments range from 1 MeV to 200 GeV incident energy. Averaging each measurement including our own over everything but target material we obtain 39 independent measurements of the deviation from theory whose distribution is normal with a mean value $-0.3 \pm 0.5\%$ and an rms spread of 3%. We conclude that Molière theory with the Fano correction is accurate to better than 1% on the average for protons. Systematic discrepancies on the order of a few percent with target thickness and/or target material cannot be ruled out at present. In particular there is some indication that the theory may be $\approx 4\%$ high for the highest-Z materials.

- **Extract from the abstract of Gottschalk's paper.**
- **Can MICE make any stronger statement?**
- ***Recently discovered a 2016 paper by Gottschalk et al. who claim comparison of G4 with Molière is better than comparison of G4 with measurements. They did that and (I think) they concluded G4 is OK for their purposes – proton therapy.***

REFERENCES (Partial)

- **G. Molière, Z. Naturforsch, 3a, 78 (1948) (in German)**
- **H.A. Bethe, Phys. Rev. 89, No. 6, 1256 (1953) (in English)**
- **U. Fano, Phys. Rev. 93, No. 1, 117 (1954)**
- **B. Gottschalk *et al.*, NIM B74 467 (1993)**

- **Also papers by:**
  - **Wentzel, Lewis, Goudsmit & Saunderson, Scott, Snyder & Scott, Kultchitsky & Latyshev, Williams**