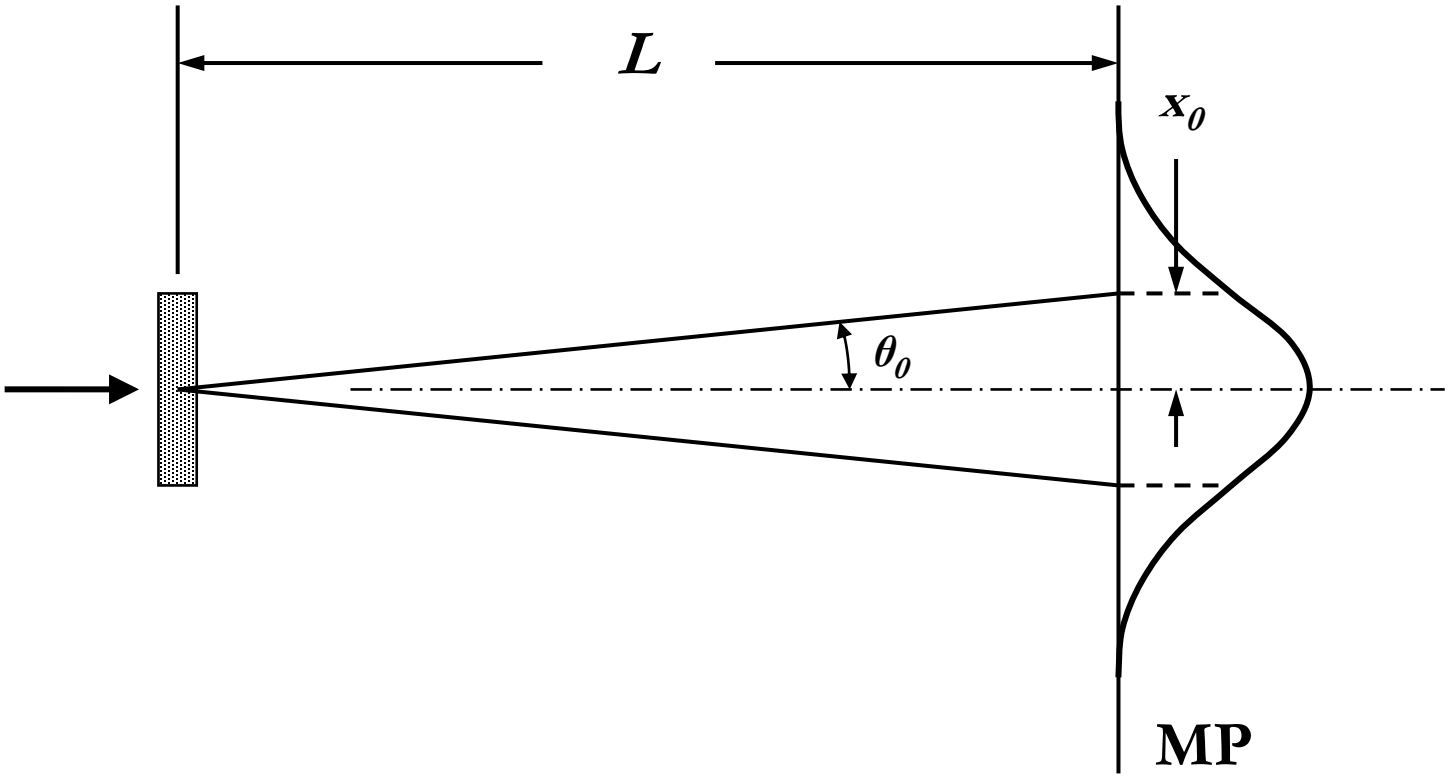
Multiple Scattering



When protons pass through a slab of material they suffer millions of collisions with atomic nuclei. The statistical outcome is a *multiple scattering angle* whose distribution is approximately Gaussian. For protons, this angle is always small so the projected displacement in any measuring plane **MP** is also Gaussian. The width parameter of the angular distribution is θ_0 . The corresponding displacement, x_0 , can easily be measured by scanning a dosimeter across the MP. The task of multiple scattering theory is to predict θ_0 given the scattering material and thickness, and the incident proton energy.

Molière Theory

Many statistical processes obey the Central Limit Theorem: the random sum of many small displacements is a Gaussian distribution. However, the displacements must all be *small ,* in a sense that can be made mathematically precise. Scattering from the screened Coulomb field of the atomic nucleus does not obey the CLT because the single scattering cross section falls off only as $\mathbf{1/\theta^4}$, too slowly. Therefore the angular distribution is approximately Gaussian for small angles but eventually tends to a 'single scattering tail' $\mathbf{\approx 1/\theta^4}$ **.**

All this was well understood by many investigators who worked on multiple scattering in the 1920's and 30's but it was Molière who in 1947 published the definitive theory, uniting the Gaussian region with the large-angle region in a precise and elegant way. He computed the distributions of both the *space* and *projected* angles for *arbitrarily thick* targets as well as *compounds and mixtures*, and produced numerical results long before the general availability of digital computers. His numerical evaluations were later improved somewhat by Bethe, who considered the overall Molière theory to be good to 1%.

His name notwithstanding, Molière was German. In his first paper, he derives an accurate formula for single scattering in the screened Coulomb field of the nucleus. The second, which uses that formula to compute multiple scattering, was his 'Habilitationsschrift' (a published work that qualified one to join the faculty) at the University of Tübingen. He thanks Prof. Heisenberg for his interest and advice.

An Early Measurement with Electrons

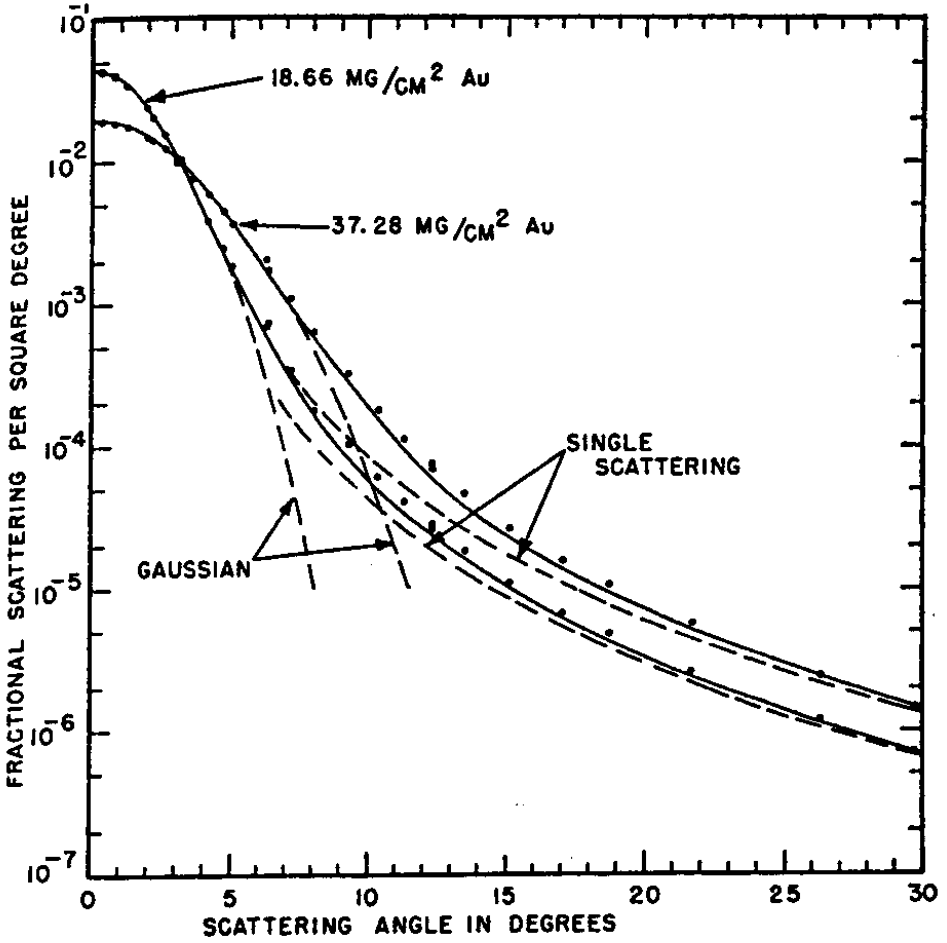


FIG. 3. Angular distribution of electrons from thick and thin gold foils from 0° to 30°. The solid line represents the theory of Molière extrapolated through the region where his small and large angle approximations give different values. The dotted lines at small angles represent the continuation of the gaussians of Fig. 1. At larger angles, the dotted line represents the single scattering contribution.

Hanson et al., 'Measurement of multiple scattering of 15.7 MeV electrons,' Phys. Rev. **84** (1951) 634-637 studied electron scattering by thin and thick foils of Be and Au. They also gave a formula for computing the width of the best Gaussian fit to the exact theory ('Hanson's formula' below). Their overall measurements agree well with Molière not only in the small angle (Gaussian) region but also in the single scattering tail. The theoretical transition between the two regions was improved by Bethe later on.

The First Measurement with Protons

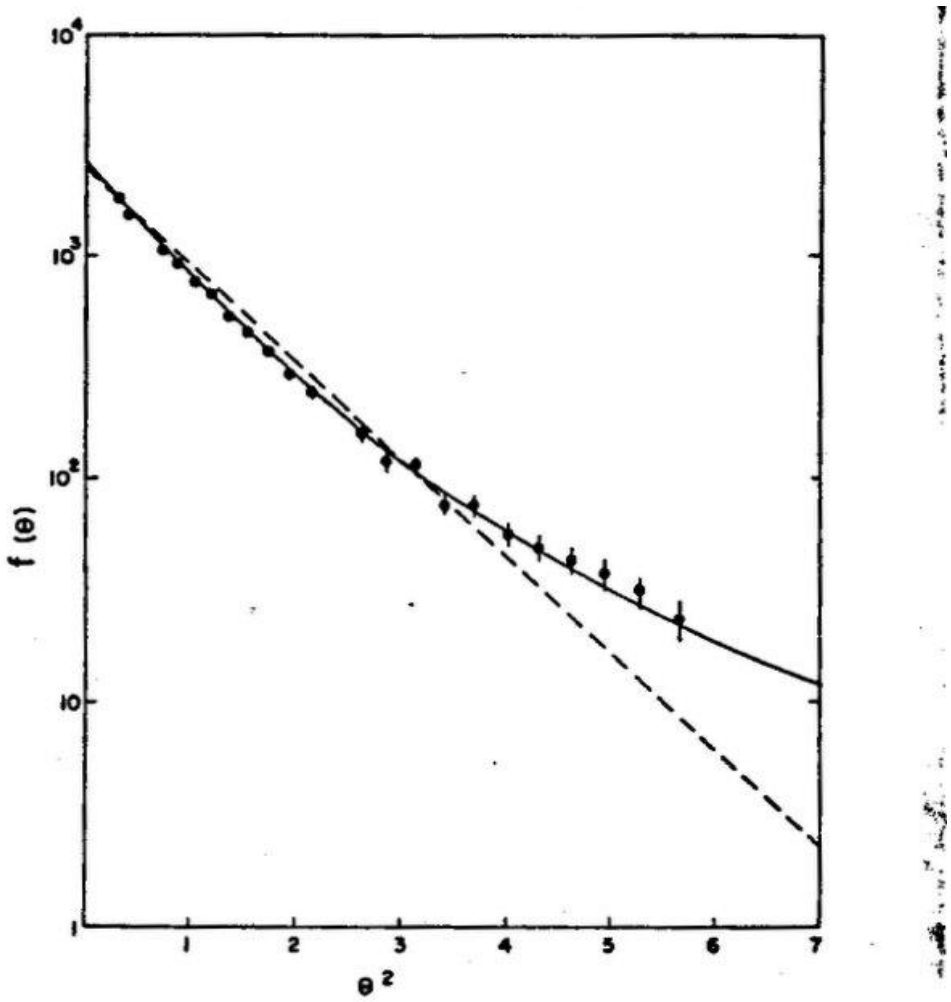
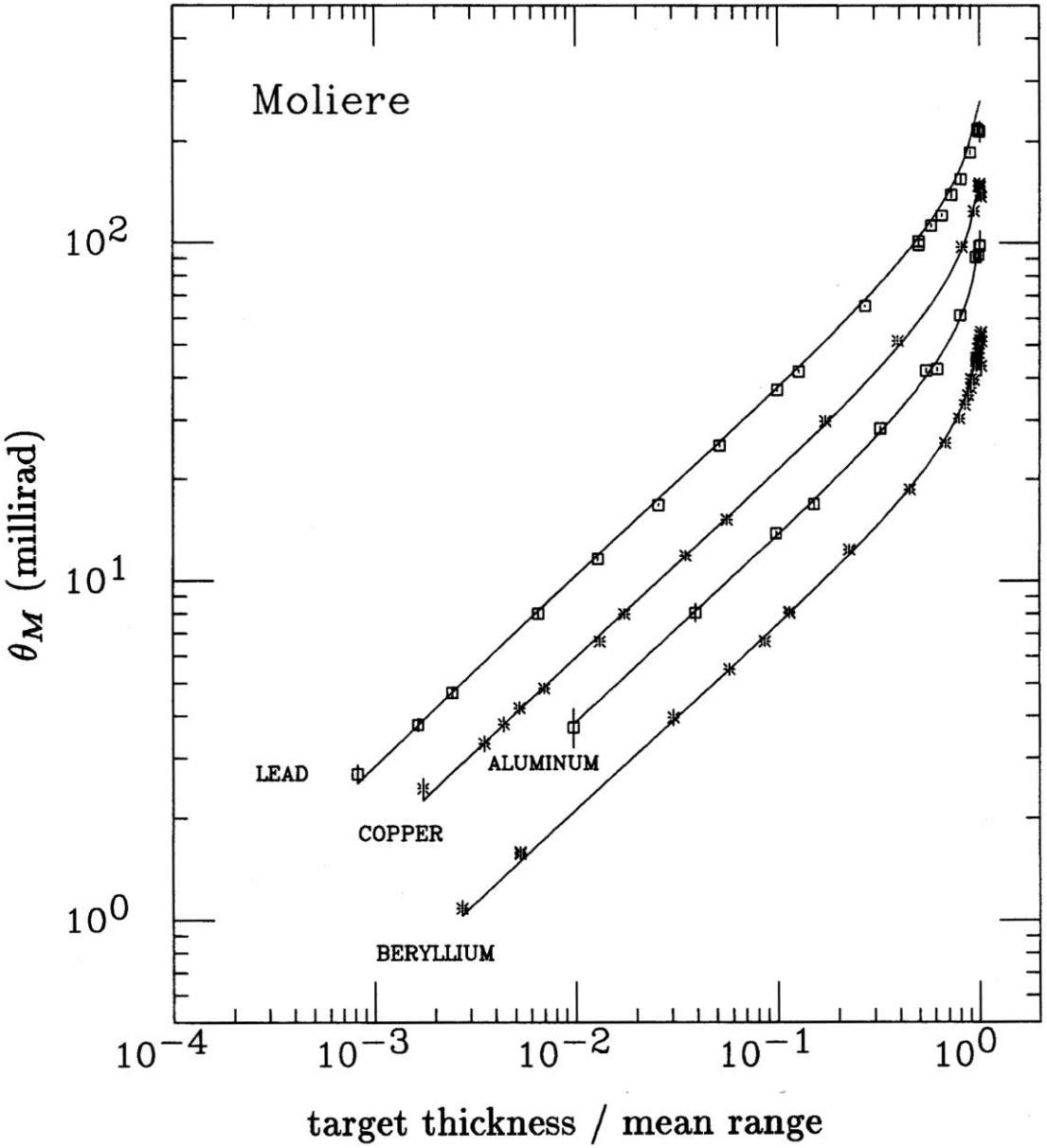


FIG. 5. Comparison of experimental data from Fig. 3 with theory. The solid line represents a normalized Molière function (adjusted with only one parameter: the absolute cross section). The dotted line represents a Gaussian curve, the zero-order term of the Molière function.

H. Bichsel, 'Multiple scattering of protons,' Phys. Rev. 112 (1958) 182-185 bombarded targets of Al, Ni, Ag and Au with protons ranging from 0.77 to 4.8 MeV from a Van de Graaff accelerator. His detector was a tilted nuclear track plate. He fitted his measurements with the Molière form at the appropriate $\boldsymbol{B}$, adjusting only the characteristic angle $\boldsymbol{\theta_0}$. The results agreed with theory to $\pm 5\%$. Bichsel went on to become a leading expert in range-energy and straggling theory and modeling the Bragg peak.

Comprehensive Test of Molière Theory



Gottschalk et al., 'Multiple Coulomb scattering of 160 MeV protons,' Nucl. Instr. Meth. B74 (1993) 467-490. Molière theory predicts the multiple scattering angle correctly over the periodic table, three decades of normalized target thickness and over two decades of angle. Compounds and mixtures (not shown) are also covered. The theory has no empirical parameters!

References

[1] G. Molière, 'Theorie der Streuung schneller geladenen Teilchen I Einzelstreuung am abgeschirmten Coulomb-Feld,' Z. Naturforschg. **2a** (1947) 133-145.

[2] G. Molière, 'Theorie der Streuung schneller geladenen Teilchen II Mehrfach- und Vielfachstreuung,' Z. Naturforschg. **3a** (1948) 78-97.

[3] H.A. Bethe, 'Molière's theory of multiple scattering,' Phys. Rev. **89** (1953) 1256-1266. Four entries in the second column (the Gaussian) of Table II are slightly incorrect (A. Cormack, priv. comm.) but the error (corrected in our programs) is at worst 1%.

[4] B. Gottschalk, A.M. Koehler, R.J. Schneider, J.M. Sisterson and M.S. Wagner, 'Multiple Coulomb scattering of 160 MeV protons,' Nucl. Instr. Meth. **B74** (1993) 467-490. We have discovered the following errors: Eq.(2) should read

$$\Xi(\chi) = \frac{1}{\pi} \frac{\chi_c^2}{(\chi^2 + \chi_a^2)^2}$$

and in Table 1 the heading α should read α^2 and $\times 10^9$ under χ_c^2 should read $\times 10^6$.

‘But it’s in German!’

Although Molière starts his paper by considering thin elementary targets, presumably for clarity, he later covers thick scatterers as well as compounds and mixtures. Both generalizations are very important for proton beam line design and dose algorithms. Early workers in the field, such as Bichsel and Scott, were well aware of these generalizations.

However, Bethe’s 1953 paper (in English) didn’t include those aspects. His remark ‘Lewis[5] has shown how the energy loss can be taken into account ...’ seems odd because Molière also shows it. In any event, Bethe was interested in other aspects of the theory, and made a number of improvements.

Some English-speaking readers apparently thought Bethe’s review was comprehensive and assumed that Molière theory only applied when the energy loss was small. ‘Effective energy’ fixes were used. Molière’s original papers were always cited, of course!

Caveat Emptor

One of the limitations of the theory (indeed, in *any* of the forms described above) is in the allowable values of B. The quantity e^b gives approximately the number of collisions suffered by the particle in traversing the foil[7]). Since the theory is statistical in nature, we cannot expect it to represent the physical situation if the number of collisions is less than about 10–20. If $e^b = 15$, then $b = 2.7$ and, from eq. (27), $B \cong 4$. Therefore, we consider only cases for which $B \gtrsim 4$. At the other extreme, b (and, hence, B) increases with the thickness t of the scattering foil. In the theory, it is assumed that the scattered particle does not undergo any energy loss in a collision. Since energy *is* lost in each collision and since the scattering cross section is a function of energy, the theory becomes inaccurate if t is large and the particle loses too much energy in the foil. We adopt as a reasonable criterion that the particle must lose less than about 20% of its initial energy in the foil. [In any event, the value of E that enters the calculation through β, as in eq. (30), should be the *mean* energy in the foil, i.e., $E = E_{inc} - \frac{1}{2}\Delta E$.] For most cases of interest, this restriction on t limits the value of B to be less than about 15.

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This paper by two well-known theorists manages to make two mistakes in the same paragraph. Molière theory *does* cover energy loss, and if a single kinematic factor is used in simpler theories, it should be the *geometric* not the arithmetic mean of the incoming and outgoing values.

Nevertheless ...

die Ergebnisse in Tabellenform mit. Nur für einige charakteristische Größen geben sie Interpolationsformeln an, die zum Vergleich mit unseren Reihenentwicklungen (§§ 7 bis 10) geeignet sind (vgl. Anm. 20, S. 92).

§ 6. Berücksichtigung des Energieverlustes

Bevor wir das Ergebnis des letzten Abschnittes weiter auswerten, wollen wir es so verallgemeinern, daß es auch dem Energieverlust der Teilchen in der Schicht Rechnung trägt. — Es sei jetzt E_0 die Energie, mit der die Teilchen auf die streuende Schicht treffen; nach Zurücklegung eines Weges l' in der Schicht sei die Energie auf einen Wert $E(l')$ abgesunken. Die Wahrscheinlichkeit dafür, daß ein Teilchen auf einem kleinen Wegstück dl' eine Einzelablenkung um einen Winkel χ innerhalb $d\chi$ erfährt, sei [analog zu (1,1) und mit I, (9,1)]:

$$w(\chi, l')\,\chi\,d\chi\,dl' = \frac{2\,\chi_c'^2(l')}{[\chi^2+\chi_a^2(l')]^2}\,\chi\,d\chi\,dl'\,. \quad (6,1)$$

Dabei ist ähnlich wie in (1,2) die Winkelkonstante

$$\chi_c'(l') = (a/k_0)\sqrt{4\pi N} \quad (6,2)$$

und der Abschirmungswinkel χ_a nach I, (9,3):

$$\chi_a(l') = (1/a\,k_0)\sqrt{1{,}13+3{,}76\,a^2} \quad (6,3)$$

(a = Thomas-Fermi-Radius) benutzt. χ_c' und χ_a sind

Molière Theory

χ_c is a characteristic single scattering angle:

$$\chi_c^2 \;=\; c_3\, t/(pv)^2$$

B characterizes target thickness (long computation):

$$B \;\propto\; \log(t/\text{mean range})$$

θ_M is analogous to θ_0:

$$\theta_M \;\equiv\; \frac{1}{\sqrt{2}}\,\chi_c\,\sqrt{B} \quad , \quad \theta' \;\equiv\; \frac{1}{\sqrt{2}}\,\frac{\theta}{\theta_M}$$

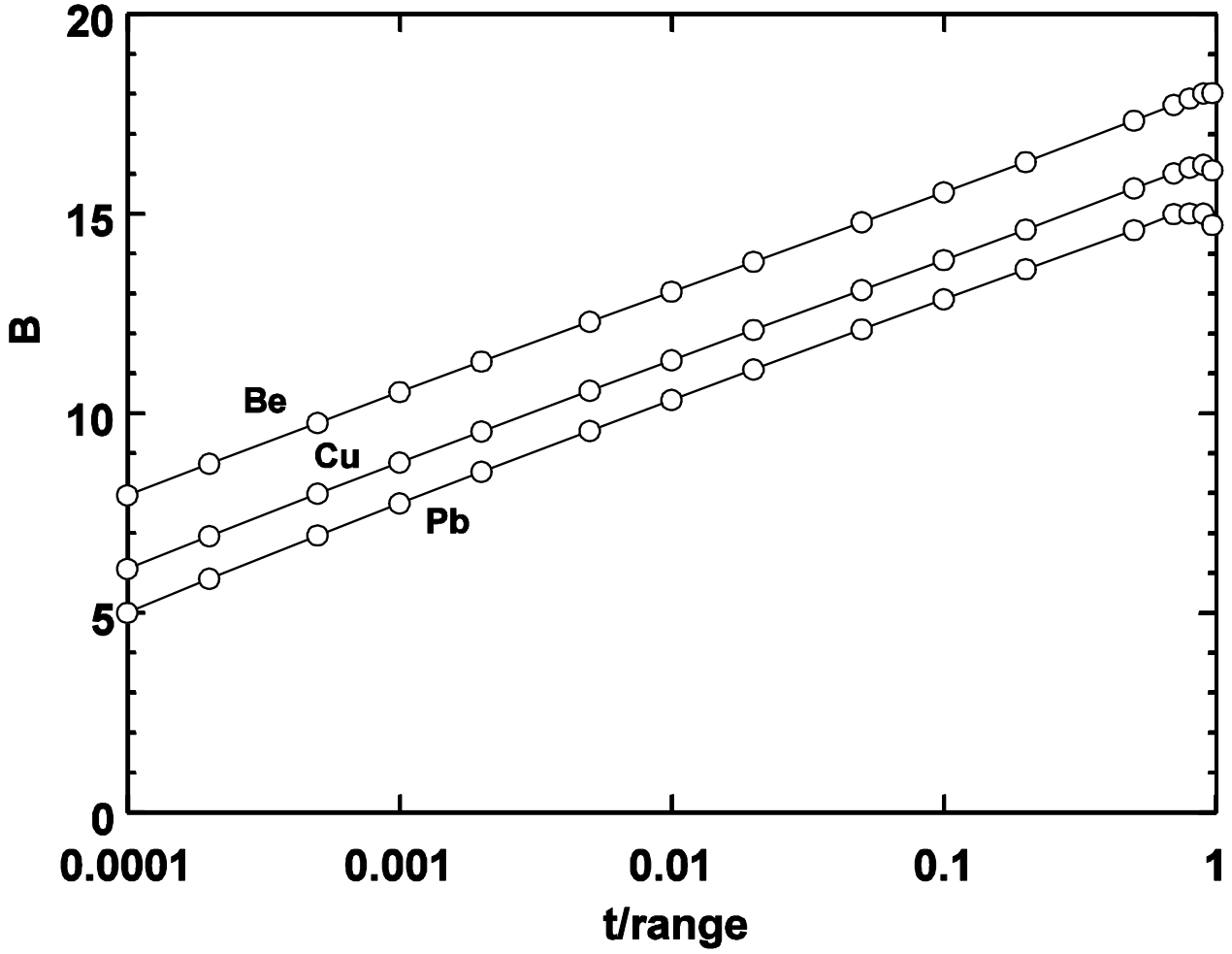
The 2D probability density is:

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

Hanson's expedient (1951):

$$\theta_0 \;\doteq\; \theta_H \;\equiv\; \frac{1}{\sqrt{2}}\,\chi_c\,\sqrt{B - 1.2}$$

Physical Interpretation of B



Molière's reduced target thickness ***B*** is proportional to the logarithm of the normalized target thickness (t/range) as this graph (Gottschalk et al. 1992, Table 1) shows. The constant of proportionality depends on the target material. Molière's ***b*** is identified by him as the natural logarithm of the effective number of collisions in the target.

The Gaussian Approximation

In **Molière** theory we first find, by a lengthy computation, a single scattering parameter χ_c and a dimensionless target thickness parameter **B**. The quantity $\chi_c\sqrt{B}$, a characteristic multiple scattering angle, is the scale factor in a PDF which consists of three terms in powers of **1/B** . The first is a Gaussian.

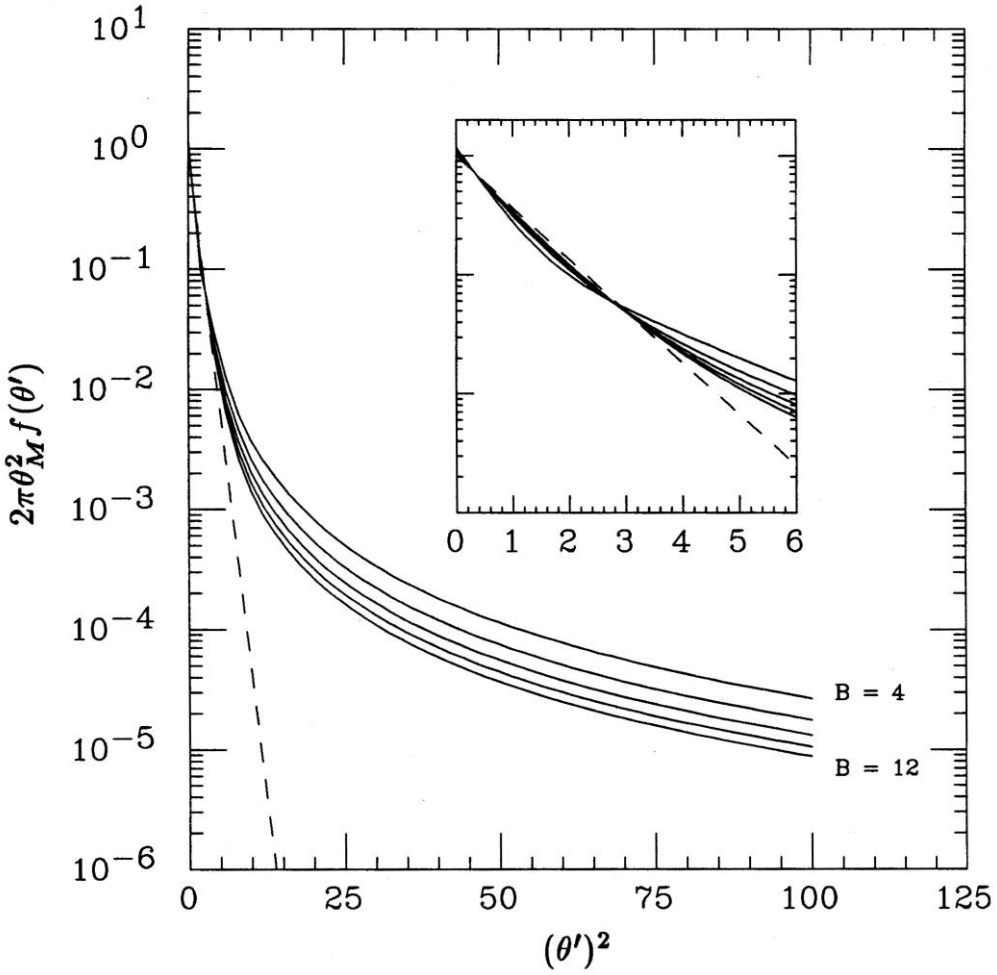
Hanson et al. (Phys. Rev. 84 (1951) 634) were the first to observe that the best Gaussian approximation is obtained, not by retaining just Molière's first term, but by using a Gaussian whose σ is a bit narrower, $\theta_0 = \chi_c\sqrt{(B-1.2)}$. This approach still requires the entire Molière computation.

Later, **V.L. Highland** (NIM 129 (1975) 497-499) fitted Molière/Bethe/Hanson theory and found

$$\theta_0 = \frac{14.1 \text{ MeV}}{pv} z \sqrt{\frac{L}{L_R}} \left[1 + \frac{1}{9} \log_{10}\left(\frac{L}{L_R} \right)\right] \qquad \text{rad}$$

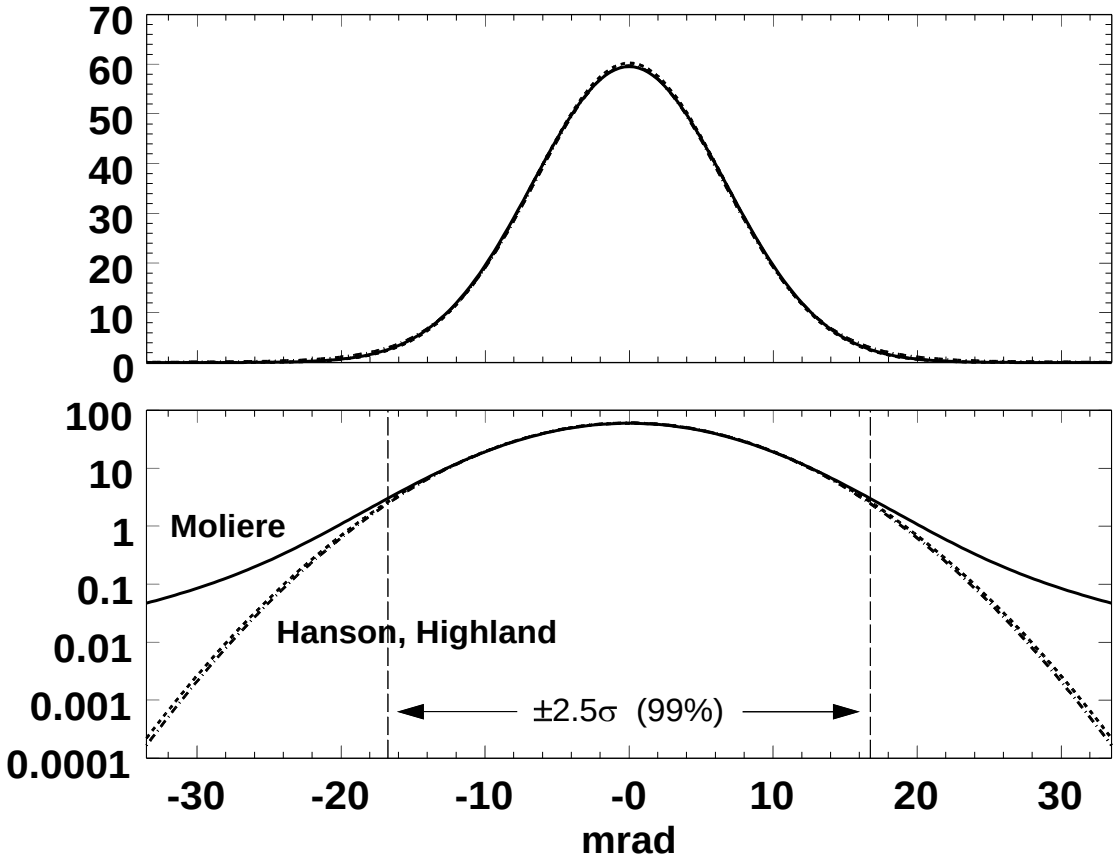
This simple formula circumvents the Molière calculation and is often used as a proxy for Molière theory in the Gaussian approximation. The scattering material is entirely represented by its radiation length L_R , which we can look up or calculate from the chemical composition. Highland's formula may be generalized to thick targets by integration but we must take the correction factor [ ] outside the integral.

Gaussian Approximation (cont.)



Molière angular distribution for various values of B, plotted so a Gaussian becomes a straight line. Shows the relative insensitivity to B, the slow approach to single scattering, and the large deviation from a Gaussian at larger angles. Inset: the dashed line is Molière's Gaussian term. The distribution at small angles is well approximated by a Gaussian, but one with a somewhat smaller characteristic width.

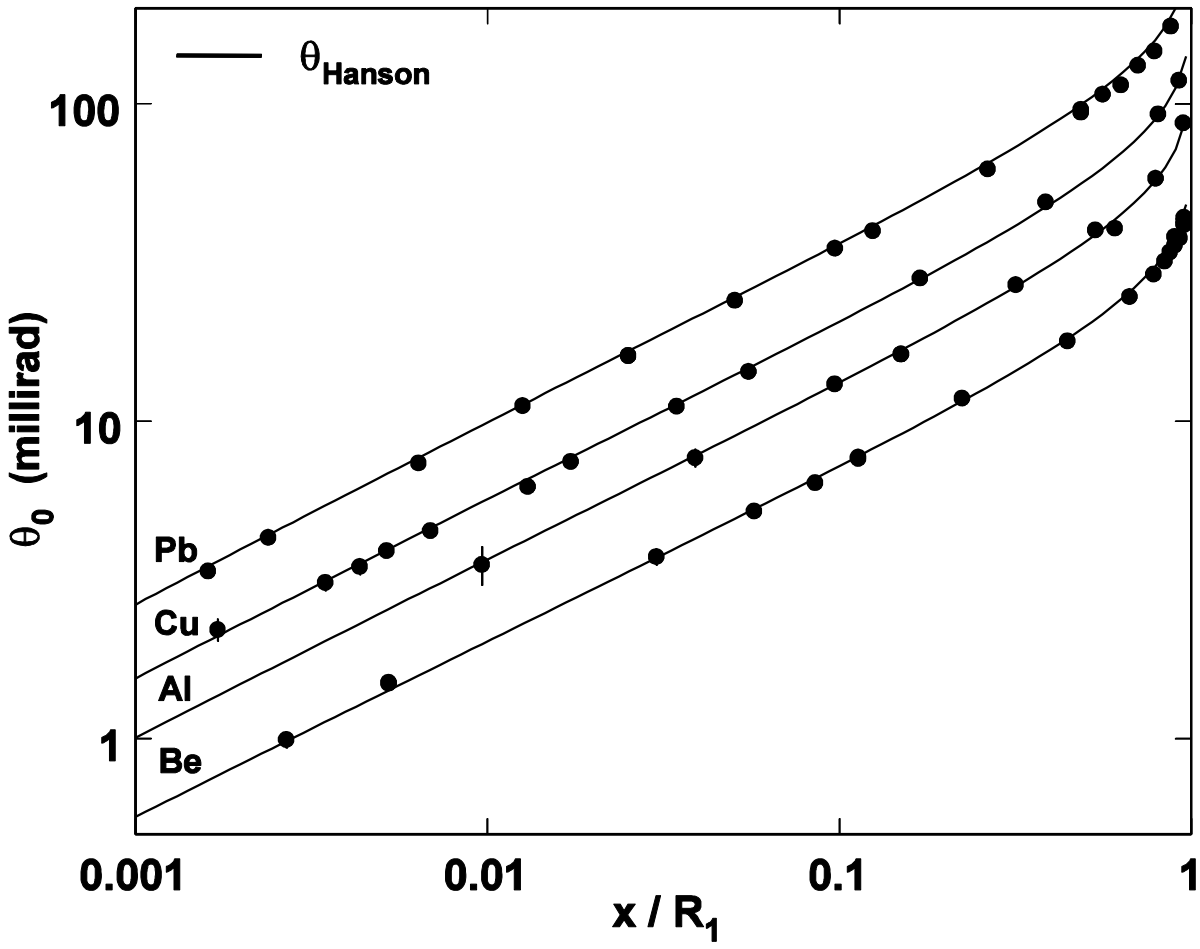
Gaussian Approximation (cont.)



Projected angle distributions for 158.6 MeV protons on 1 cm of H_2O ($\sigma \approx 6.7$ mrad). On a linear plot the Molière/Fano distribution is indistinguishable from Gaussians using the Molière/Fano/Hanson or Highland θ_0. However, it peels away at 2.5σ , and at 5σ is more than 100× higher.

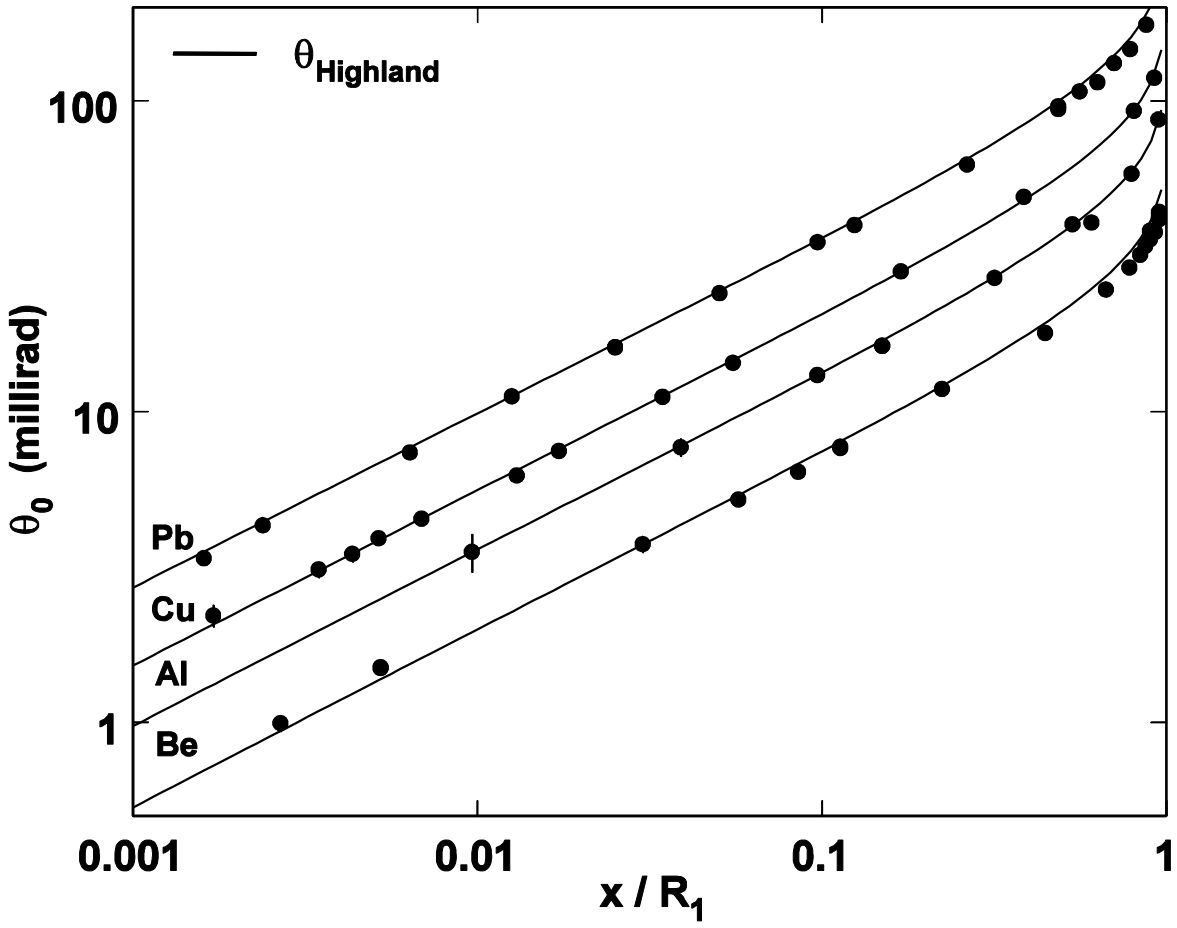
We need the correct distribution only if we are looking for rare anomalous events, not if we are estimating the resolution of a spectrometer.

Molière/Fano/Hanson (θ_{Hanson})



Same paper as before, but measurements are fit with a Gaussian. We regard Molière/Fano/Hanson as the gold standard in the Gaussian approximation, and will try to construct a scattering power which, when integrated over target thickness, will reproduce it.

Generalized Highland ($\theta_{Highland}$)



Same data, Gaussian fit. Agreement of this simple formula is almost as good as θ_{Hanson} (full calculation). (Be is slightly high because Highland fitted Molière/Bethe/Hanson instead of Molière/Fano/Hanson.)

Comparison of Approximate Formulas

Rossi 1941: $$\theta_0 = \frac{15}{pv}\sqrt{\frac{L}{L_R}}$$

Hanson 1951: $$\theta_H \equiv \frac{1}{\sqrt{2}}\left(\chi_c\sqrt{B-1.2}\right)$$

Highland 1975: $$\theta_0 = \frac{14.1\ \text{MeV}}{pv}\, z\sqrt{\frac{L}{L_R}}\left[1 + \frac{1}{9}\log_{10}\left(\frac{L}{L_R}\right)\right]$$

For 160 MeV protons incident on 1 g/cm^2 of each material:

material	L/R %	L/L_R %	Hanson mrad	Highland ÷ Hanson	Rossi ÷ Hanson
beryllium	4.62	1.53	4.68	1.016	1.354
Lexan	5.40	2.41	6.04	1.016	1.318
water	5.67	2.77	6.56	1.012	1.302
brass	3.73	8.13	12.11	0.994	1.203
lead	2.73	15.70	17.37	0.995	1.162

Highland's Formula for Thick Targets

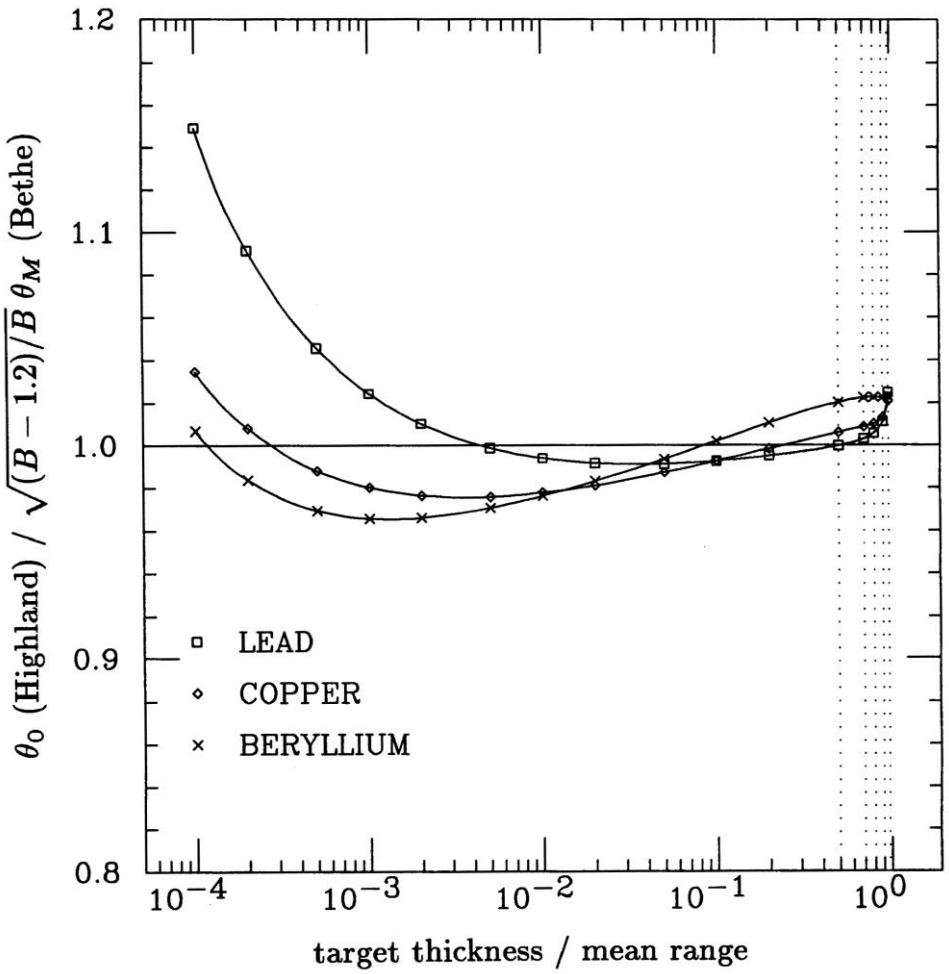
Unlike the full Molière theory, Highland's formula as originally given applies only to thin targets, as shown by the telltale factor $\boldsymbol{pv}$. We extended it to moderately thick and very thick targets. In the first case it is frequently good enough to replace $\boldsymbol{pv}$ by its geometric mean : $\boldsymbol{pv} \rightarrow \boldsymbol{p_1 v_1 p_2 v_2}$ where 1,2 refer to the incoming and outgoing proton. For very thick targets, however, it is necessary to integrate over the target thickness, assuming, of course, that the proton range-energy relation is known.

$$\theta_0 \;=\; 14.1\; z \left[1 \;+\; \frac{1}{9}\;\log_{10}\!\left(\;\frac{L}{L_R}\;\right)\right] \times \left[\int_0^L \left(\frac{1}{pv}\right)^2 \frac{dt'}{L_R}\right]^{1/2} \qquad \text{rad}$$

Notice that we have taken the logarithmic correction factor *out of the integral*. It is evaluated for the target *as a whole*. Without this step (if we think of evaluating the integral numerically) the answer would get ever smaller as dt' became smaller. Other arbitrary measures could be used, such as fixing the integral step size. This is the one we prefer, and the one used in comparing Highland's formula with data in our paper.

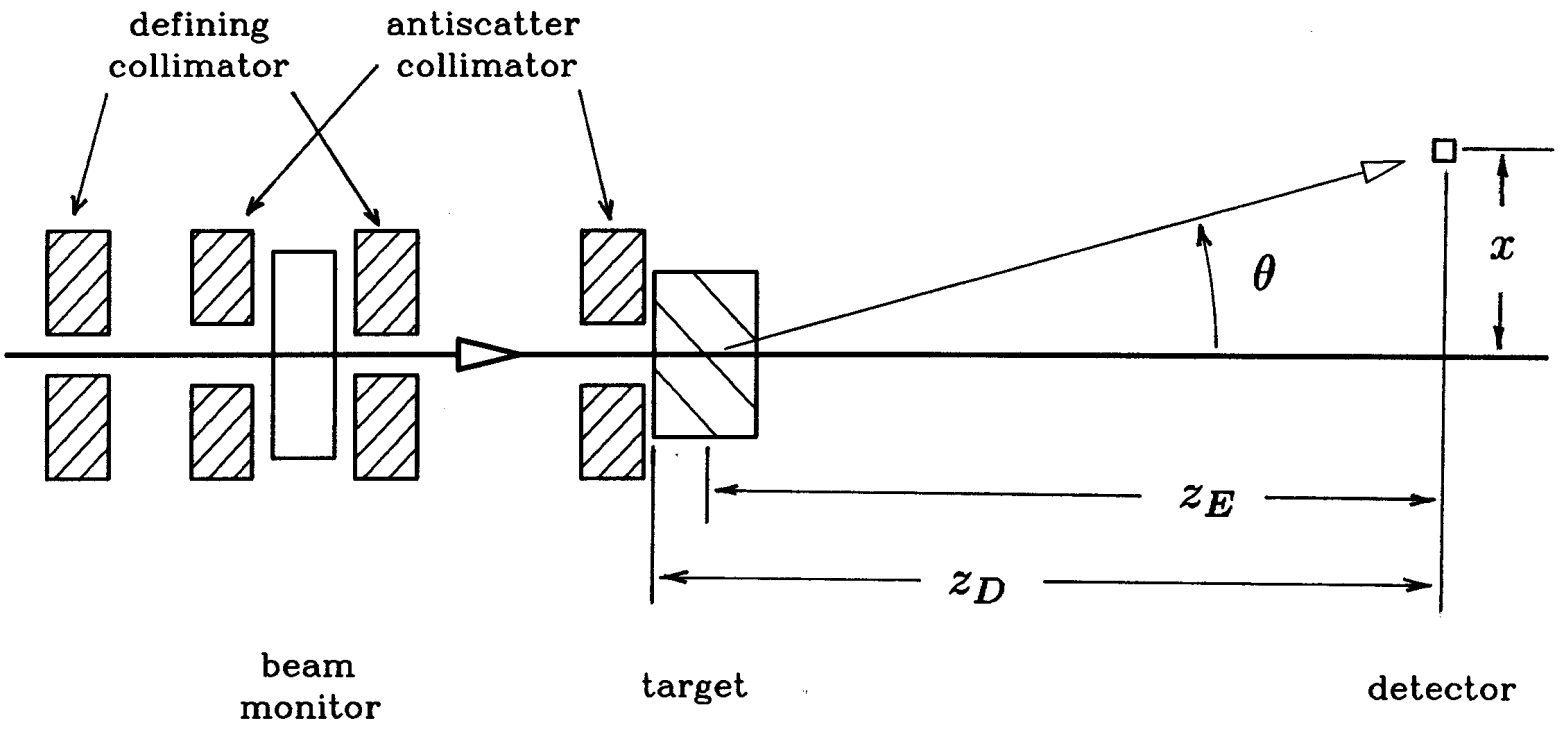
Because of the way the integrand depends on depth, it is efficient to divide the target by equal *ratios* rather than equal *steps* when evaluating the integral numerically.

Accuracy of Highland's Formula



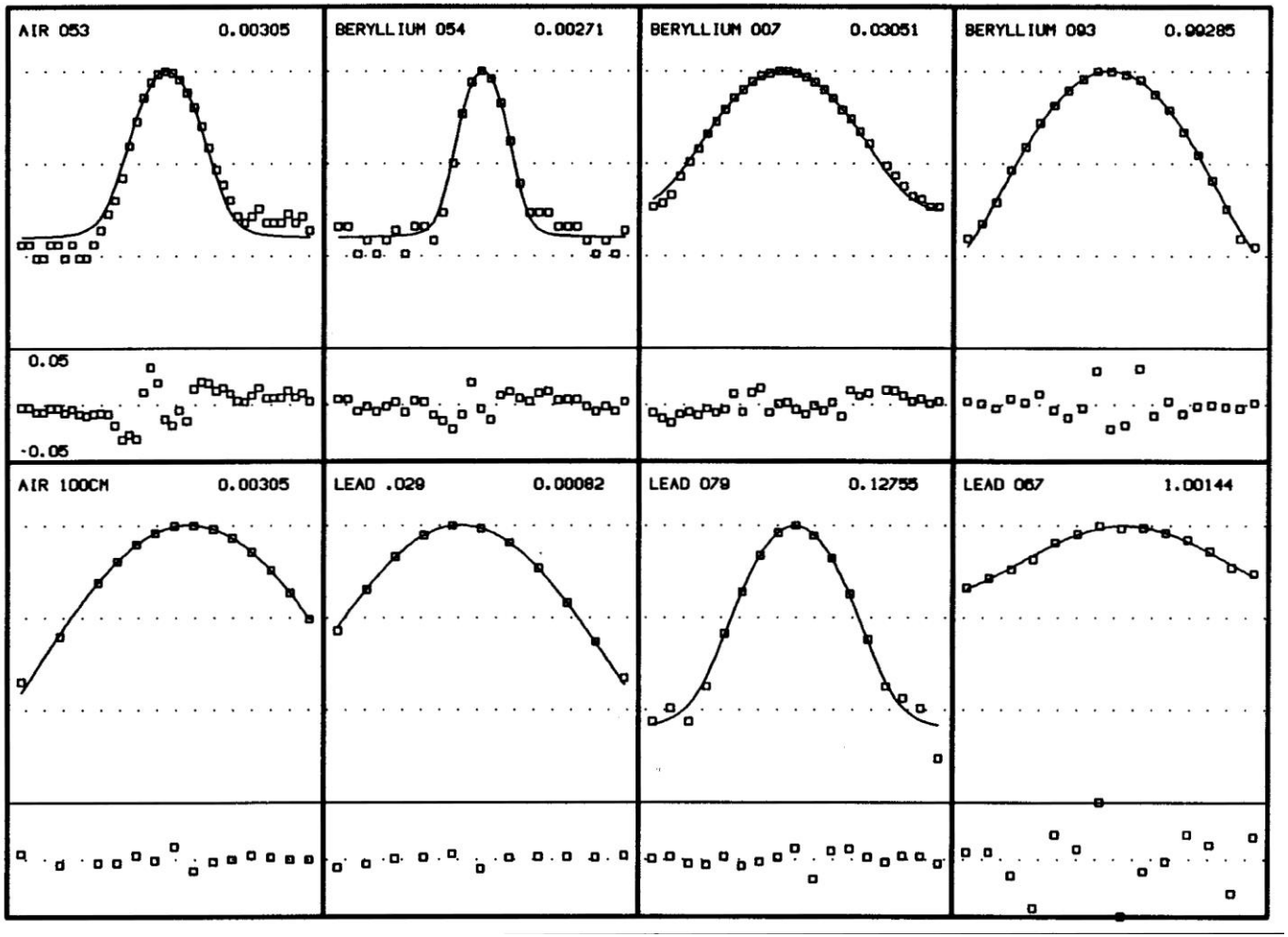
This shows the accuracy of Highland's formula, as generalized to thick targets by us., as a parameterization of Hanson's formula applied to the Bethe form of Molière theory. It is good to $\pm 5\%$ as claimed by Highland except for the thinnest points for lead, which are outside his allowed range.

The HCL Experiment 1967-1987



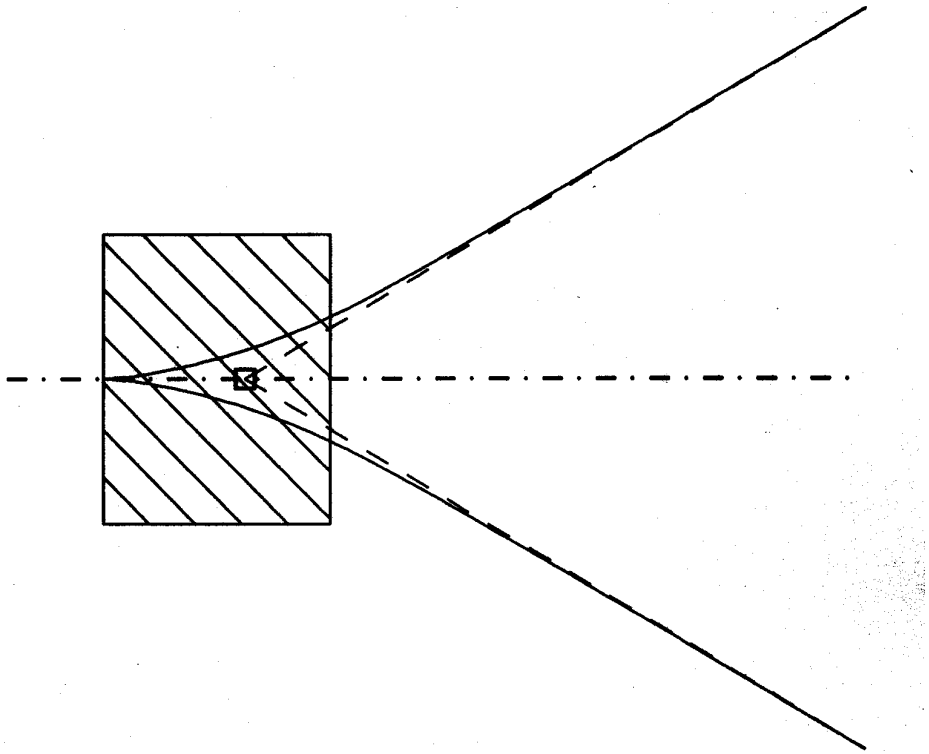
A well collimated beam of protons scattered in the target and fell on a measuring plane where the transverse dose distribution was measured by a diode. The data were fit to obtain θ_M and θ_0 and the corresponding 'air' (target out) angle was subtracted in quadrature. In converting to angle, the virtual source position was obtained from theory. Over 20 years, 115 different thicknesses and materials were measured with steadily more automated methods but the same basic principle.

Typical Data and Fits



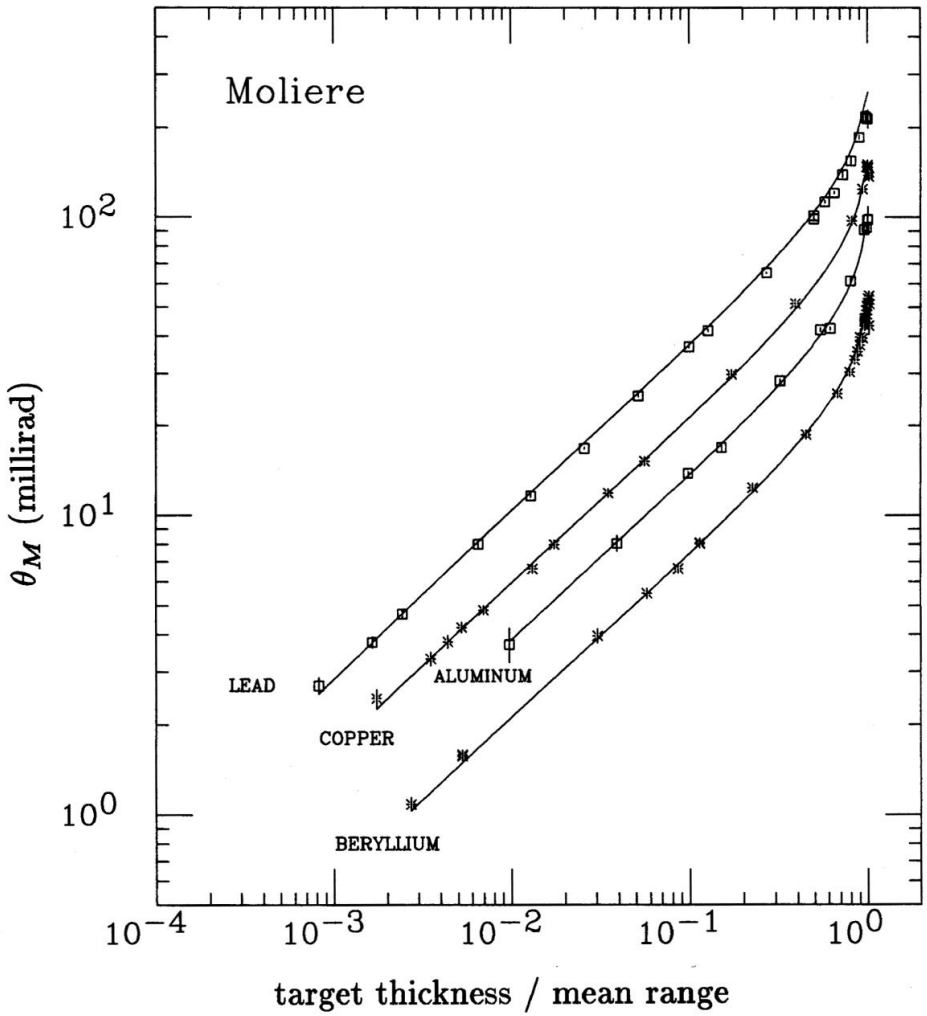
Top: air run and thin through thick Be runs. Bottom: air run an thin through thick Pb runs. Top right each frame: normalized target thickness. Main frame: measured data in a semilog plot. Bottom window each frame: fit residual in a linear ±5% window.

The Virtual Point Source



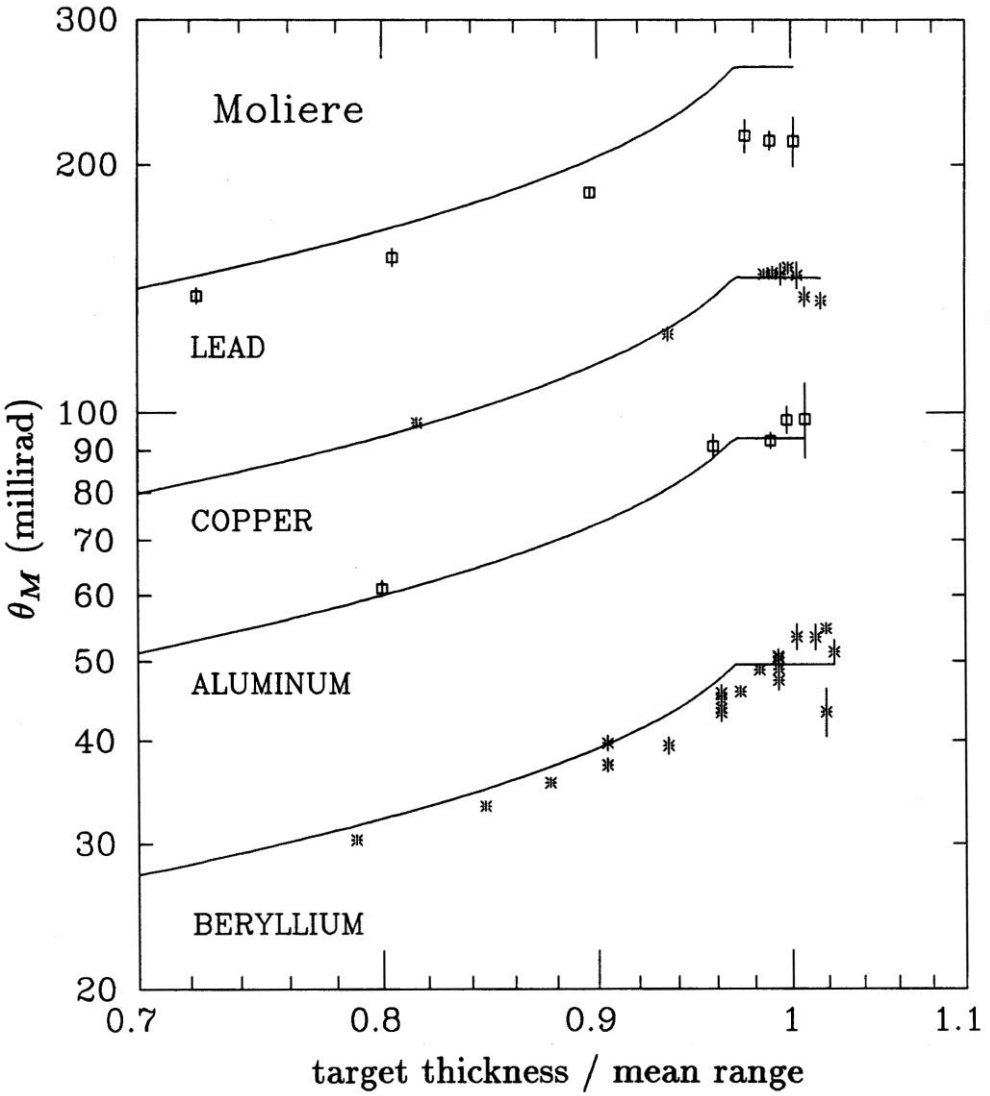
Because of the rather short throw in the HCL experiment (to conserve signal), it was necessary, especially for the thicker targets, to estimate where the protons were coming from. We called this the 'effective origin' of scattered particles. The proper term per ICRU Report 35 (1984) is 'virtual point source'. The diagram suggests how it may be calculated. First, we need an expression for the size parameter of the scattered beam as a function of ***z***. Then we extrapolate from two sufficiently distant points. Details may be found in the paper and will be covered in a later lecture.

Overview of HCL Results

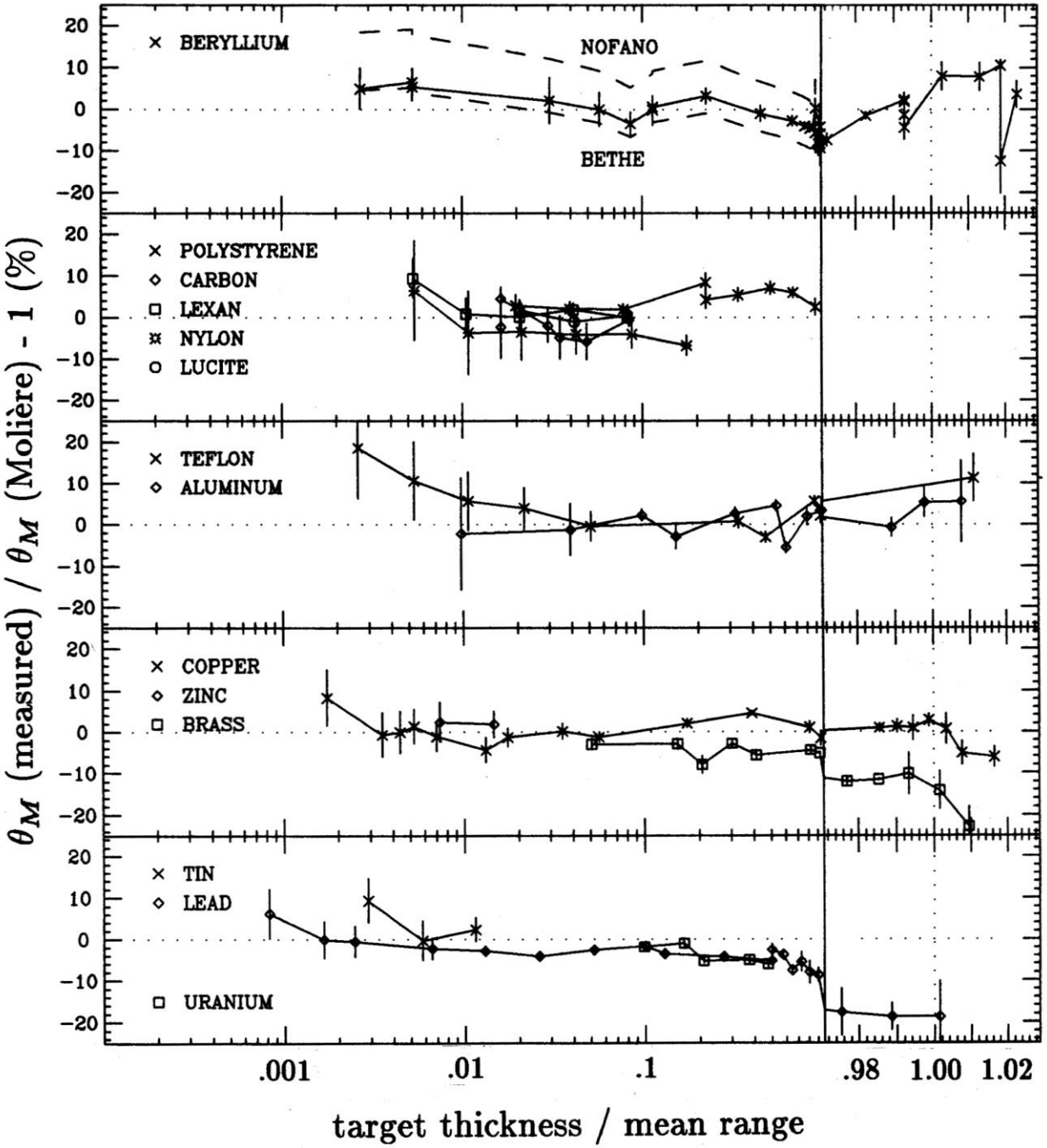


This graph shows the sweep of Molière theory. With *no empirical parameters* it predicts the characteristic multiple scattering angle from Be to Pb over three decades of normalized target thickness and two decades of multiple scattering angle.

Behavior Near End-of-Range



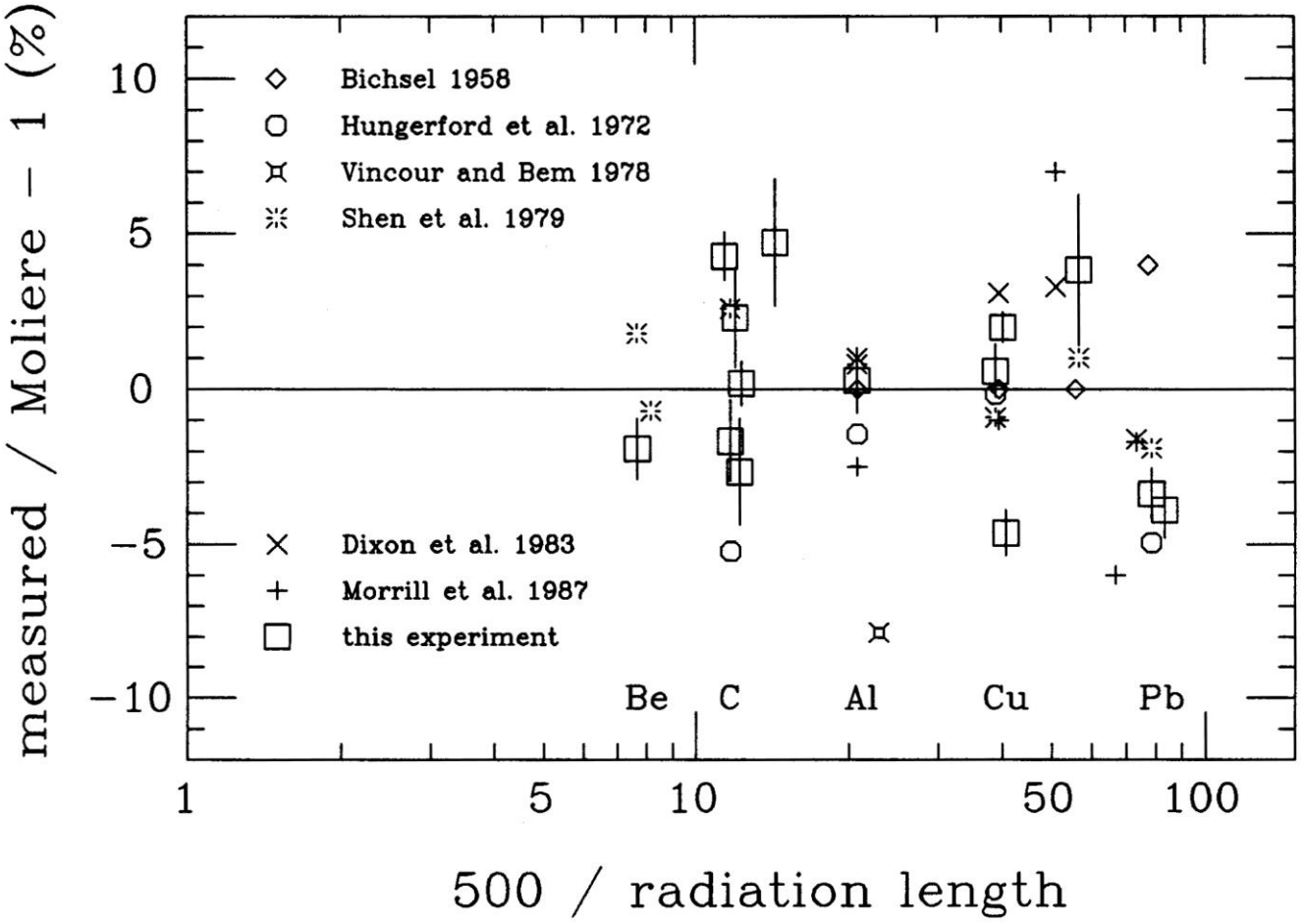
At the Bragg peak, because of range straggling, there is no longer any strong correlation between depth and proton energy, and the multiple scattering angle appears to saturate.



A Closer Look

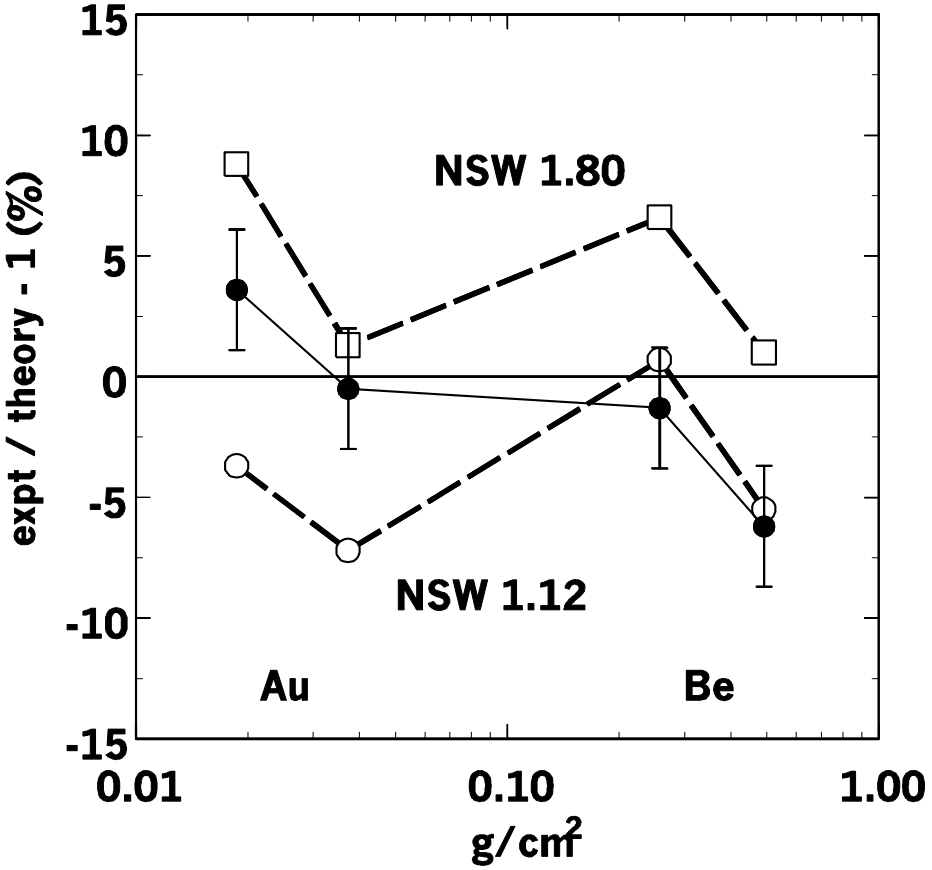
This graph compares the HCL results to Molière theory on a linear scale in a ±25% window. We use the 'Fano correction' for scattering by atomic electrons throughout, but it only matters for Be. The region (target > 0.97× mean range) is separated and plotted to a different scale. Excluding those points, the mean error overall is –0.5 ±0.4% with an rms width of 5%. The same comparison for Highland's formula (not shown) gives –2.6 ±0.5% with a width of 6%. The Lynch and Dahl formula gives very similar results.

Grand Summary



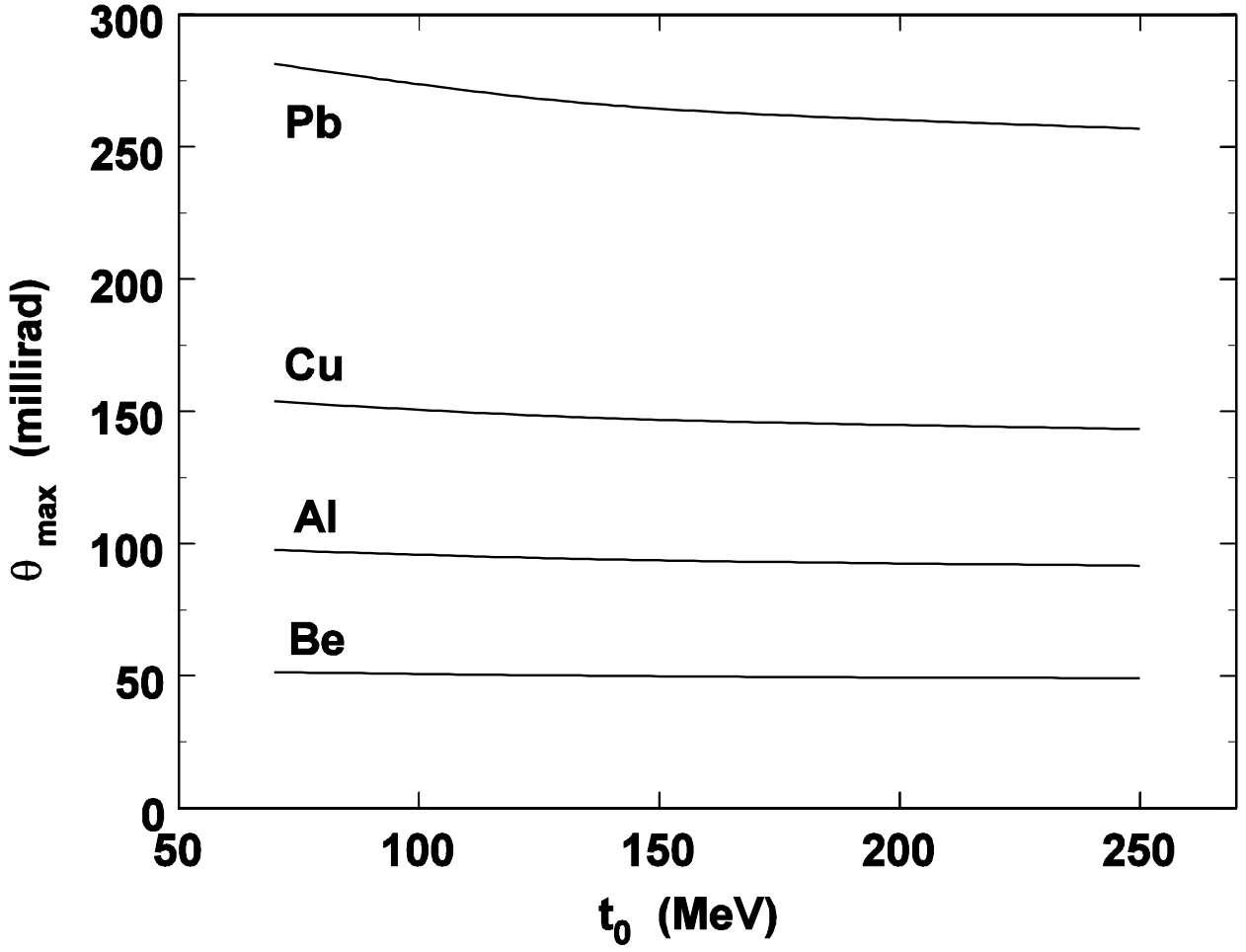
We reviewed and in some cases reanalyzed the six previous proton studies. Some of those claimed Molière's theory was wrong, others were not aware of his generalization to thick targets. The summary, above, is plotted to an arbitrary abscissa with each experiment averaged over everything but target material. The experiments ranged from 1 MeV to 200 GeV. The mean is –0.3 ±0.5% (!) with an rms spread of 3%.

A Competing Theory



The theory of Nigam, Sundaresan and Wu (NSW) is claimed by them to be more correct on theoretical grounds and to give better agreement with the electron data of Hanson et al., where they used only *two* of the *four* measurements. NSW theory is of the Molière form but more complicated, and has an empirical parameter. This graph shows the comparison with *all* of Hanson's data as computed by Scott (Rev. Mod. Phys. **35** (1963) 231). NSW theory is worse for *either* value of their parameter.

A Curious Fact



... first drawn to my attention by Andy (who else?) is that the *maximum* scattering angle from any material, the angle which obtains at (0.97× mean range), is very nearly independent of incident energy. Looking at Pb, it's impossible to get more than 280 mrad $\approx 16^{O}$ from protons, justifying the small angle approximation.

7.4 Fortran Function Theta0

`Theta0` incorporates all the formulas and procedures of this Chapter. Before calling it you must initialize the range-energy functions:

```
i = InitRange('\BGWARE\DATA\ICRU49.RET')
                  ...
mode = 'MOLIERE '
thetaM = Theta0(mode,tgm,t2,matl,bb)
```

Input parameters are `MODE` which is a code (8 characters) for the scattering theory; `TGM`, the target g/cm^2; `T2`, the *outgoing* kinetic energy (MeV) and `MATL` which is a code for the target material (20 characters). Output, in addition to the function value, is `BB`, Molière's B. There is also a `COMMON` block

```
COMMON/Extras/nn,alfasq,chi0sq,chiasq,chicsq,b
```

which allows the calling program to access the Molière parameters. It need not be used otherwise. `NN` is the number of target slabs used for integration; the others are obvious. `Theta0` has extensive comments: see these for details.

In addition to computing the characteristic angle for Molière theory and its variants and approximations, `THETA0.FOR` also contains a subprogram for computing the multiple scattering angular distribution. This routine, `BetheF`, uses Bethe's tables [5]. To see how it is used consult `InitFscat` in `CSI.FOR`. Note that `Fscat` is initialized by `MAIN` only once, using typical target parameters *viz.* LEAD, 1 g/cm^2, 160 MeV. These are only used to compute B, on which $f(\theta)$ depends very weakly (Figure 7.5).

```
 task                              ?  STACK              THETA0
 material                          ?  WATER
 scattering theory                 ?  HIGHLAND
 thickness (g/cm2)                 ?     1.000
 outgoing energy (MeV)             ?   130.000
 theta0 (radian)                   = 0.007784
 task                              ?  THETA0
 material                          ?  WATER
 scattering theory                 ?  HIGHLAND    HANSON
 thickness (g/cm2)                 ?     1.000
 outgoing energy (MeV)             ?   130.000
 theta0 (radian)                   = 0.007724
 task                              ?  THETA0
 material                          ?  WATER
 scattering theory                 ?  HANSON      ROSSI
 thickness (g/cm2)                 ?     1.000
 outgoing energy (MeV)             ?   130.000
 theta0 (radian)                   = 0.010013
```

Combining Scatterers

In beam line design we frequently need to compute the net multiple scattering angle from (say) a sheet of plastic followed by a sheet of lead, or some even more complicated set of 'homogeneous slabs'.

Molière theory *does not apply* to a sheet of plastic followed by a sheet of lead. (It *would* apply to a fine mixture of plastic and lead!) However, we can find each characteristic angle by itself (taking energy loss into account) and add them in quadrature:

$$\theta_0^2 = \theta_{01}^2 + \theta_{02}^2 + \cdots + \theta_{0N}^2$$

That this procedure is, strictly speaking, *incorrect* is easily seen. Divide a scatterer made of a single material into halves. Their quadratic sum will always be too small by ~3%, as can also be seen directly from Highland's formula. The error is worse, the more you divide the scatterer.

Nevertheless, addition in quadrature works well enough in practice, perhaps because in common engineering situations one of the slabs will dominate.

A better method suggested by Lynch and Dahl (Nucl. Instr. Meth. **B58** (1991) 6-10) is not practical for beam line design, essentially because it does not allow us to compute slabs separately. The entire issue of *mixed slabs* is rather complicated, and will be covered later.

Summary

The Molière theory of multiple scattering applies to compounds and mixtures, and target thicknesses up to ~97% of the mean range. It has no adjustable parameters. It is at least accurate as available experiments (a few percent).

Highland's approximation to the characteristic angle of the best Gaussian fit is nearly as good as Hanson's formula based on the full theory, and far easier to evaluate. For thick targets, it must be integrated. For targets of intermediate thickness one can replace pv by $(p_1 v_1 p_2 v_2)^{1/2}$.

In beam line design, finite slabs can be combined to sufficient accuracy by adding their characteristic angles in quadrature.

High-Z materials (lead) scatter far more than low-Z materials (water, plastic). We will make use of this to design contoured scatterers compensated for energy loss or range modulators compensated for scattering angle.