

Scattering Power

arXiv:0908.1413v1 [physics.med-ph] 10 Aug 2009

and

Med. Phys. 37(1) (2010) 352-367

We thank N. Kanematsu, U. Schneider and M. Hollmark for discussions of their work and L. Urban (CERN) for providing test data on the step size dependence of Geant4.

We thank Harvard University, the Physics Department, and the Lab for Particle Physics and Cosmology for ongoing support.

You can get a copy of the article by Googling arXiv and following links.

Questions

What is scattering power (T) ?

Why do we need it ?

What happens if we try to derive T directly ?

What is the single scattering correction ?

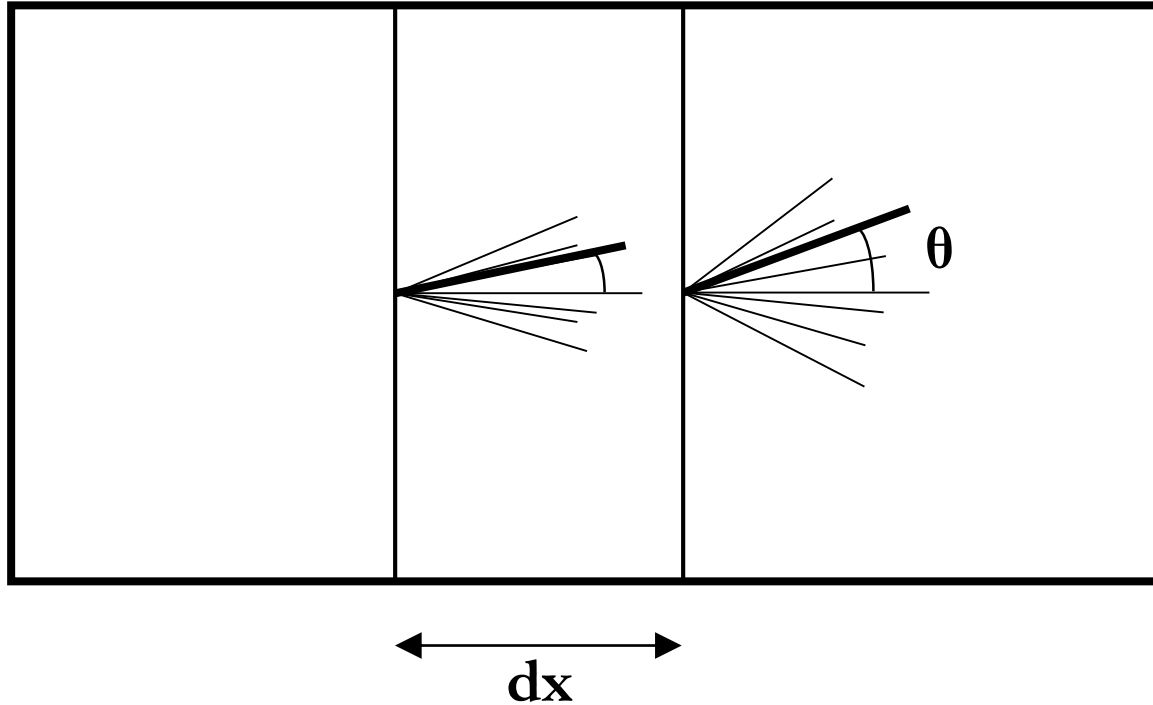
What is the correct theory of multiple Coulomb scattering in the Gaussian approximation ?

How can we use that to derive the correct form of T ?

How can we parameterize that to obtain a simple formula for T ?

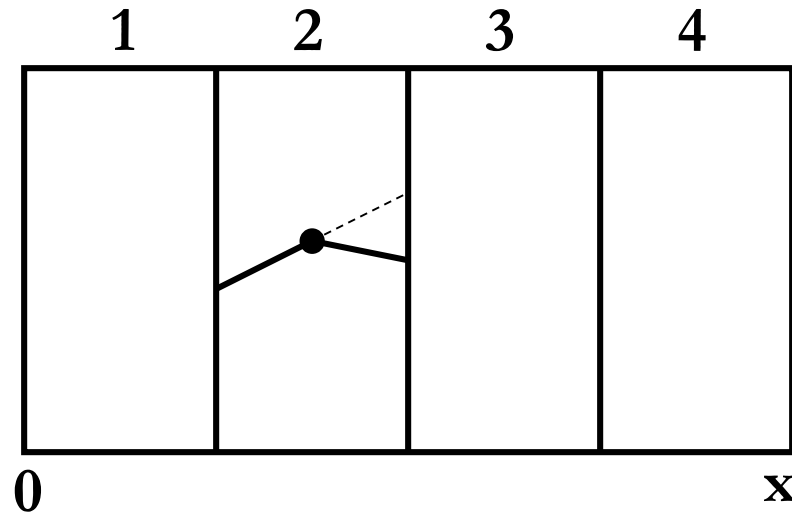
In practical problems, does the formula for T make any difference ?

What is scattering power ?



$$T \equiv \frac{d \langle \theta^2 \rangle}{dx}$$

Monte Carlo Transport



In dosimetry all practical Monte Carlos are *condensed history* MC's. The target geometry is divided into small *steps*.

Given incoming positions, slopes, energy, we estimate an *interaction point*.

At that point we compute the ms *deflection* $\Delta < \theta^2 > = T(\tilde{x}_2) \Delta x_2$

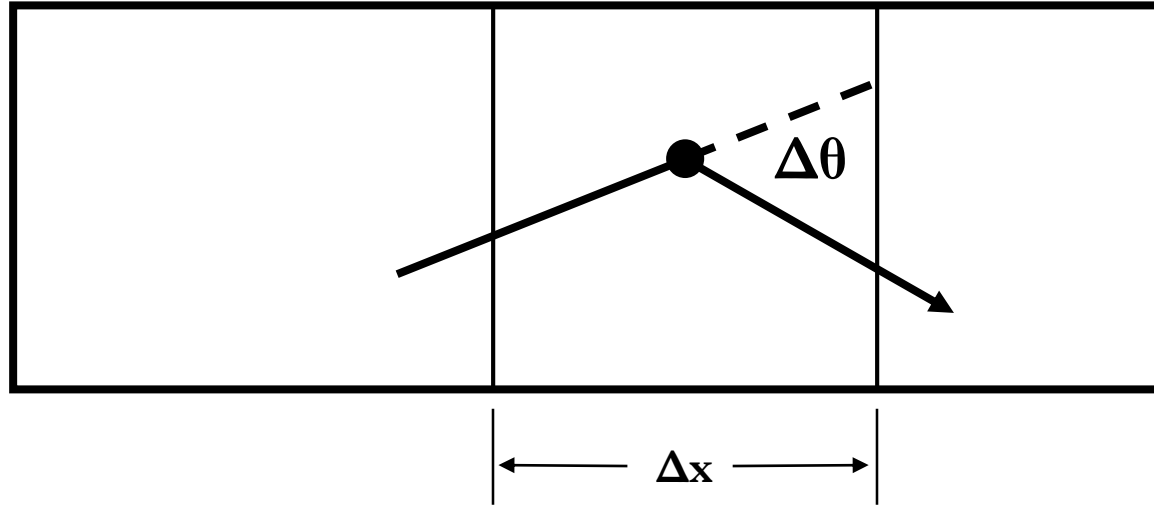
We use that as the rms of a distribution from which we pick a random deflection.

We project to the next boundary and compute outgoing *positions, slopes, and energy*.

We repeat for all steps and 10^6 protons ('histories').

We accumulate the distribution of y at x and find its rms width.

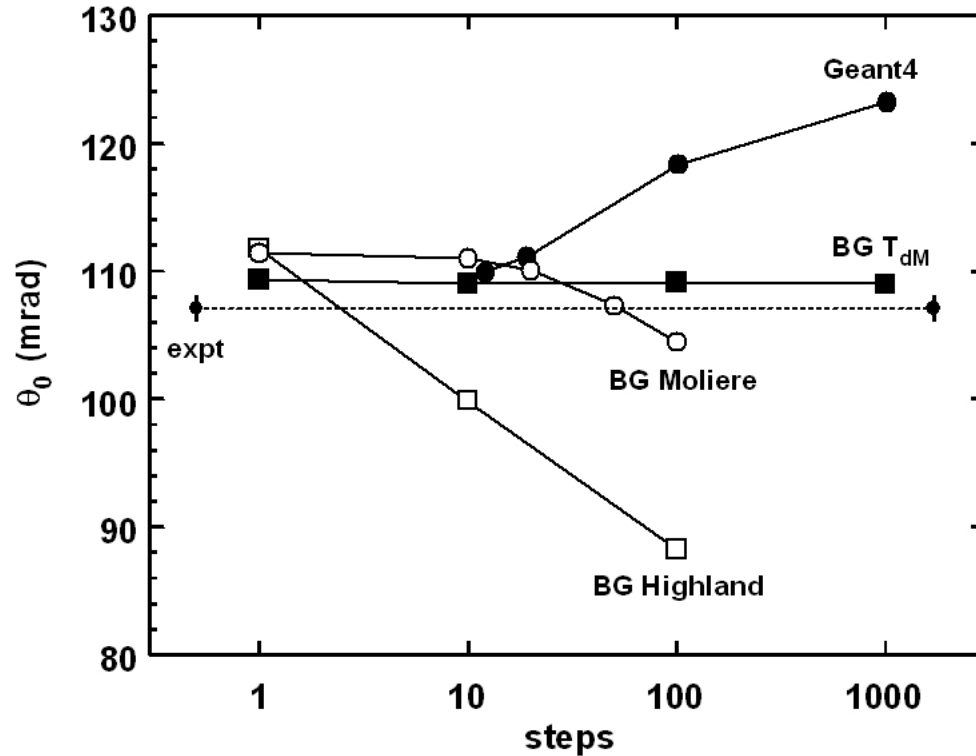
Integrating MCS in a Monte-Carlo



Method 1: treat Δx as an MCS problem *de novo* (respecting p_v , of course). Compute the parameters of a probability distribution function (PDF) and pick $\Delta\theta$ at random using that PDF. This method usually does not converge (Geant4 ?) (Note: Molière should converge but only if we do it exactly which is very slow.)

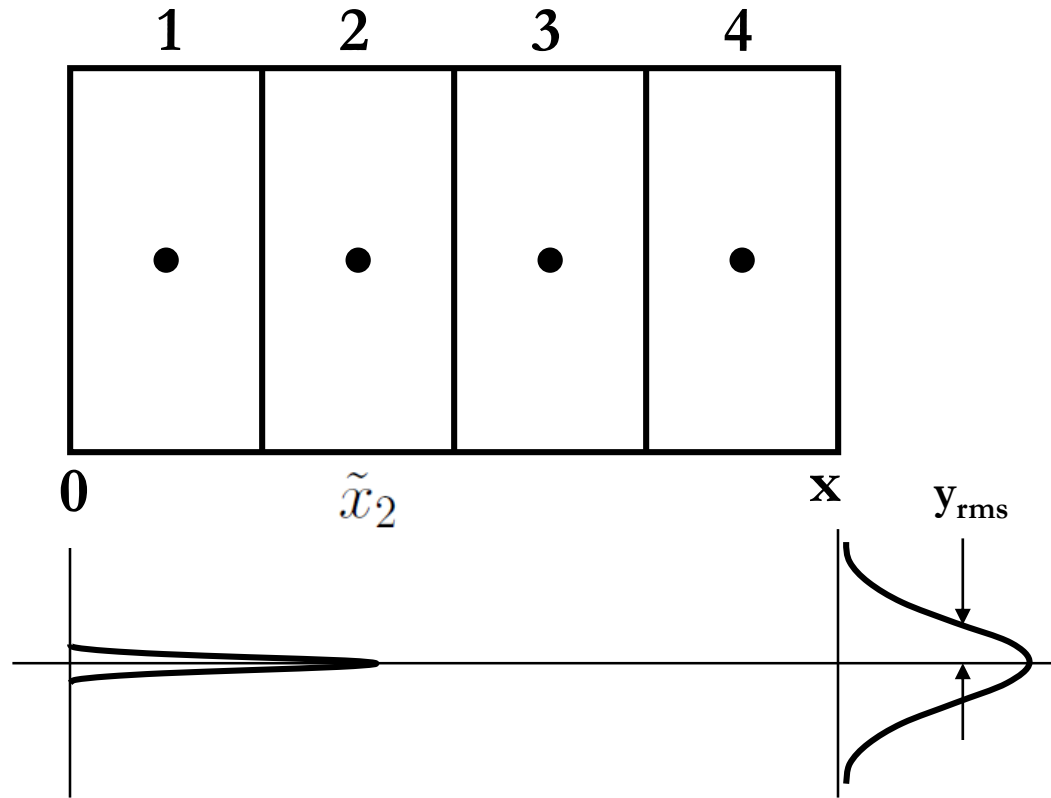
Method 2: use a ‘scattering power’ function $T \equiv d\langle\theta^2\rangle/dx$. Compute $\sigma = \langle\theta^2\rangle^{1/2} = (T \Delta x)^{1/2}$ and pick $\Delta\theta$ at random from a *Gaussian* PDF having that σ . This method converges by construction, but may be quite wrong depending on your choice of $T(x)$ (MCNPX ?). The Gaussian approximation is built in.

Convergence Studies



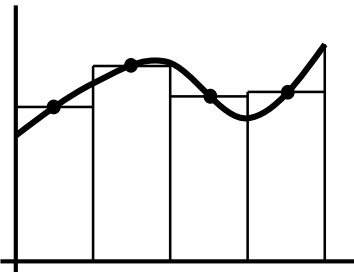
σ of the outgoing angular distribution when 158.6 MeV protons enter 20.196 g/cm² (1.78 cm) of Pb, as a function of the number of steps in a Monte Carlo calculation. 'BG' curves from BG toy Monte Carlo. Geant4 curve by courtesy of L. Urban. Experimental point from Gottschalk et al., NIM B74 (1993) 467-490 .

Deterministic (Fermi-Eyges) Transport



$$\langle y^2 \rangle = \int_0^x (x - x')^2 T(x') dx'$$

$$\approx \sum_{i=1}^N (x - \tilde{x}_i)^2 T(\tilde{x}_i) \Delta x_i \quad \text{midpoint rule}$$



What is scattering power, really ?

Unlike stopping theory, which begins with stopping power - dE/dx , multiple scattering theory does not flow naturally from a differential description. The reason is profound: we can speak of energy loss even in an atomic monolayer, but not of multiple scattering.

But we need a differential description to do proton transport.

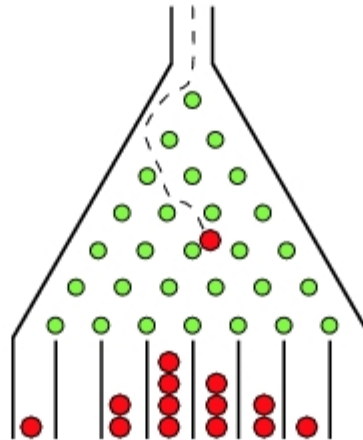
Therefore we seek *a posteriori* a differential description of Molière/Fano/Hanson theory: a function T which, when integrated, will reproduce the correct theory for a single slab to a sufficiently good approximation.

$$\langle \theta^2 \rangle = \int_0^x T(x') dx'$$

T is necessarily approximate. Some formulas are more accurate and/or more useful than others.

Having found a T that works well for single slabs we may hope that it works for mixed slabs, but we cannot know for sure. There is no accurate theory, and there are no experimental data. Monte Carlo is not a test!

Galton Board



The Galton board, also known as a quincunx or bean machine, is a device for statistical experiments named after English scientist Sir Francis Galton. It consists of an upright board with evenly spaced nails (or pegs) driven into its upper half, where the nails are arranged in staggered order, and a lower half divided into a number of evenly-spaced rectangular slots. The front of the device is covered with a glass cover to allow viewing of both nails and slots. In the middle of the upper edge, there is a funnel into which balls can be poured, where the diameter of the balls must be much smaller than the distance between the nails. The funnel is located precisely above the central nail of the second row so that each ball, if perfectly centered, would fall vertically and directly onto the uppermost point of this nail's surface (Kozlov and Mitrofanova 2002). The figure above shows a variant of the board in which only the nails that can potentially be hit by a ball dropped from the funnel are included, leading to a triangular array instead of a rectangular one.

The Single Scattering Correction

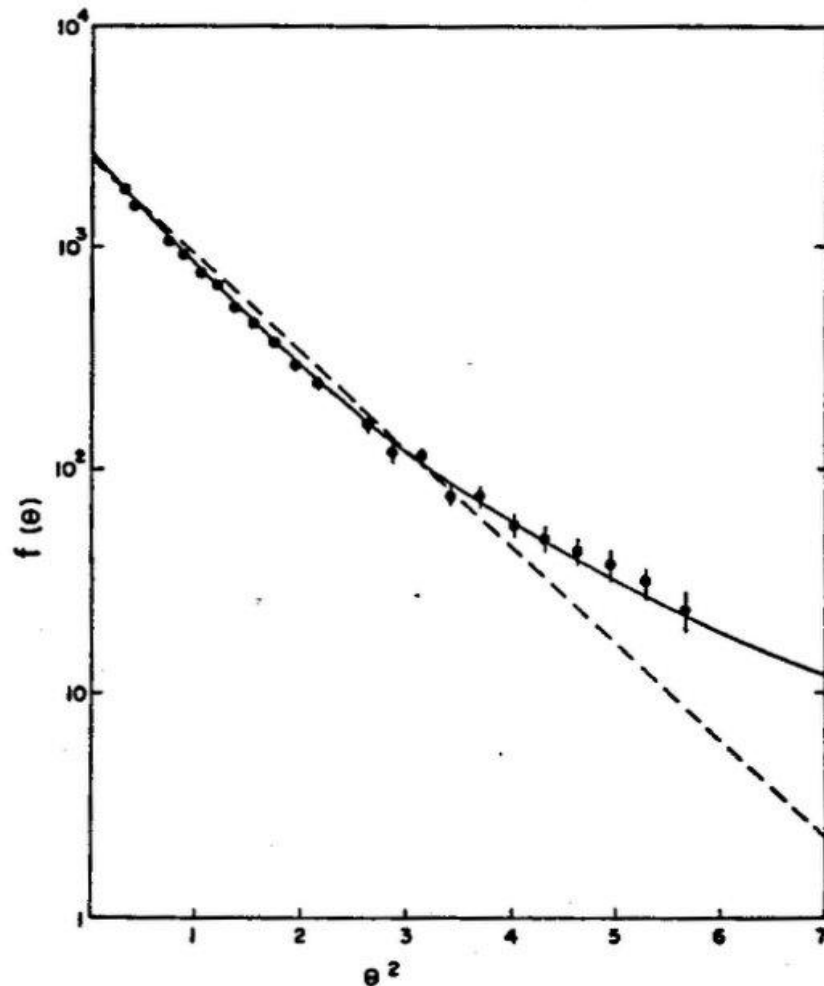


FIG. 5. Comparison of experimental data from Fig. 3 with theory. The solid line represents a normalized Molière function (adjusted with only one parameter: the absolute cross section). The dotted line represents a Gaussian curve, the zero-order term of the Molière function.

H. Bichsel, Phys. Rev. 112 (1958)
182-185

He bombarded targets of Al, Ni, Ag and Au with protons ranging from 0.77 to 4.8 MeV, Van de Graaff accelerator. Graph shows the Gaussian core and the start of the single scattering tail.

The competition between them, as you increase target thickness, affects the rate of increase of the Gaussian width. This effect, a natural part of the full theory, becomes the 'single scattering correction' when we try to write down a scattering power.

Rossi's Derivation

Rossi first gives a simplified Rutherford derivation of the single scattering probability, per unit target thickness and per unit solid angle, from an unscreened point charge, namely

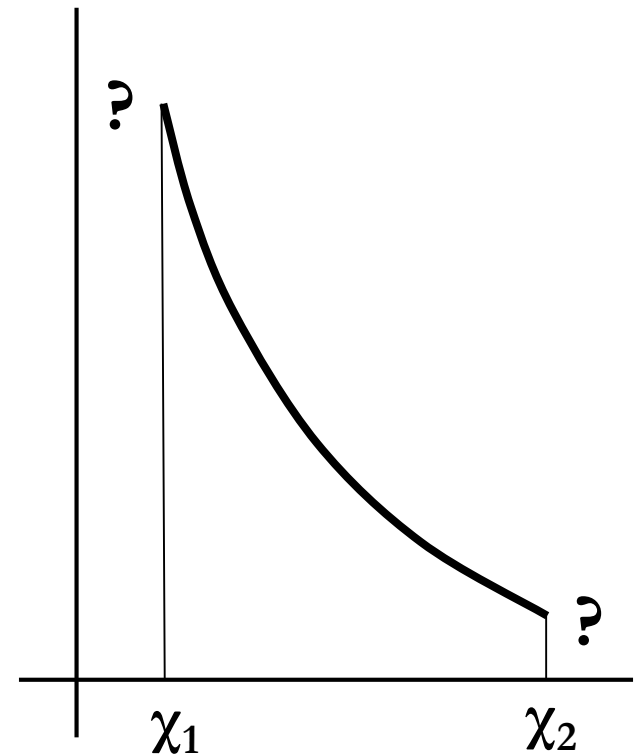
$$\Xi(\chi) d\Omega dx = 4 N r_e^2 \frac{\rho Z^2}{A} \left(\frac{m_e c^2}{pv} \right)^2 \frac{1}{\chi^4} d\Omega dx$$

$1/\chi^4$ breaks down for distant collisions (very small scattering angle) because the nucleus is screened by electrons. That happens near

$$\chi_1 = 1.13\alpha Z^{1/3} \left(\frac{m_e c^2}{pc} \right)$$

It also breaks down for very close collisions (large scattering angle) because the nucleus is not a point charge. That happens near

$$\chi_2 = \frac{2}{\alpha A^{1/3}} \left(\frac{m_e c^2}{pc} \right)$$



Rossi's Derivation (cont.)

Rossi now assumes that the mean squared angle at $(x + dx)$ equals its value at x plus the mean squared angle of scattering in dx . *This step is equivalent to assuming the MCS process is exactly Gaussian.* It leads to

$$d\overline{\Theta^2} = dx \int_0^{2\pi} \int_{\chi_1}^{\chi_2} \chi^2 \Xi(\chi) d\Omega_\chi$$

He then defines

$$\Theta_s^2 \equiv \frac{1}{\rho} \frac{d\overline{\Theta^2}}{dx} = \frac{1}{\rho} \int_0^{2\pi} \int_{\chi_1}^{\chi_2} \chi^2 \Xi(\chi) d\Omega_\chi$$

Later, Brahme called this quantity the mass scattering power T/ρ and made the analogy with mass stopping power S/ρ .

Note that in Rossi, x is expressed in g/cm^2 : his x is our ρx . Absorbing ρ in x or other quantities such as X_0 becomes very inconvenient when dealing with mixed slabs. Instead of doing that we simply regard ρ and other material properties as piecewise constant functions of depth x (cm).

Rossi's Derivation (cont.)

To do the integral in closed form one must assume some simple behavior for Ξ below χ_1 and above χ_2 . Rossi does this two different ways. The less accurate, which unfortunately became known as the 'Rossi formula', assumes that Ξ is 0 below χ_1 and above χ_2 . Then the integral is easy, and with the aid of

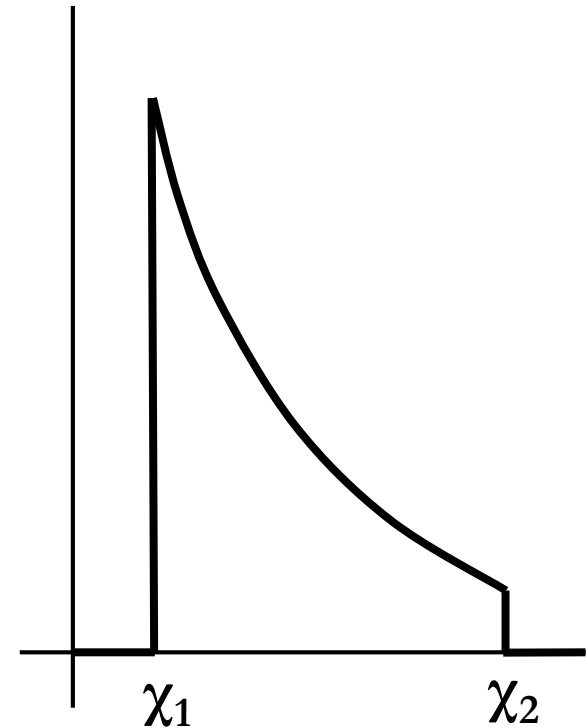
$$E_s \equiv \left(\frac{2\pi}{\alpha} \right)^{1/2} m_e c^2 = 15.0 \text{ MeV}$$

one eventually finds (in our notation):

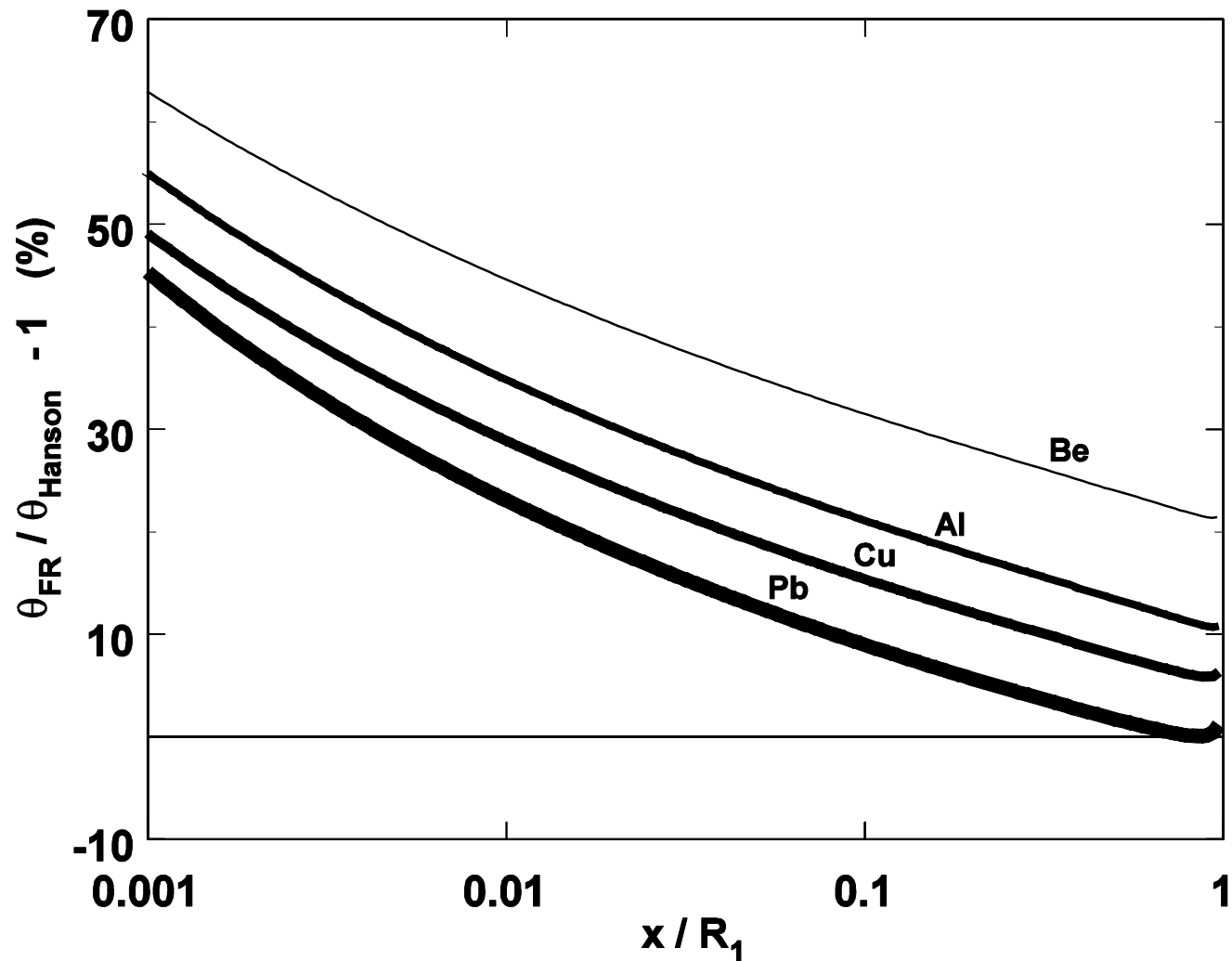
$$T_{\text{FR}} = \left(\frac{E_s}{pv} \right)^2 \frac{1}{X_0}$$

X_0 is the radiation length of the material. To find the net MCS angle in a finite slab, we must integrate T_{FR} over x , taking into account the decrease of pv (momentum \times speed) as the protons slow down:

$$A_0 = \langle \theta^2 \rangle = \int_0^x T(x') dx'$$



The Fermi-Rossi Scattering Power T_{FR}



T_{FR} is simple but it does not work very well. Here we compare its integral with the right answer. θ_0 is far too large for thin targets, and it has the wrong material dependence.

Rossi's Derivation (cont.)

Rossi later makes the more reasonable assumption that $\Xi(\chi) \approx 1/(\chi^2 + \chi_1^2)^2$ below χ_1 . The integral is a bit harder but still analytic :

$$T_{\text{IC}} = \alpha N r_e^2 \left(\frac{E_s}{pv} \right)^2 \frac{\rho Z^2}{A} \left\{ \log \left(1 + \left(\frac{\chi_2}{\chi_1} \right)^2 \right) - 1 + \left(1 + \left(\frac{\chi_2}{\chi_1} \right)^2 \right)^{-1} \right\}$$

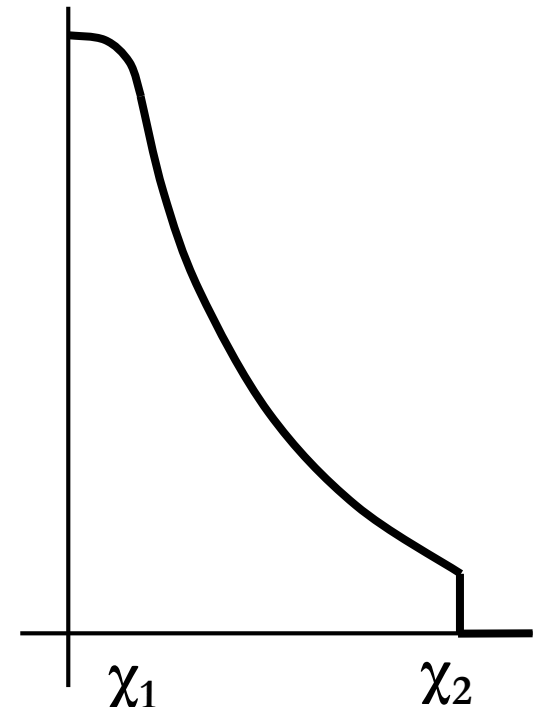
This is the scattering power given in ICRU Report 35 (1984) except that the form given there *only applies to electrons*. For protons it can be simplified by introducing a 'scattering length' X_S defined by

$$\frac{1}{\rho X_S} \equiv \alpha N r_e^2 \frac{Z^2}{A} \left\{ 2 \log(33219 (AZ)^{-1/3}) - 1 \right\}$$

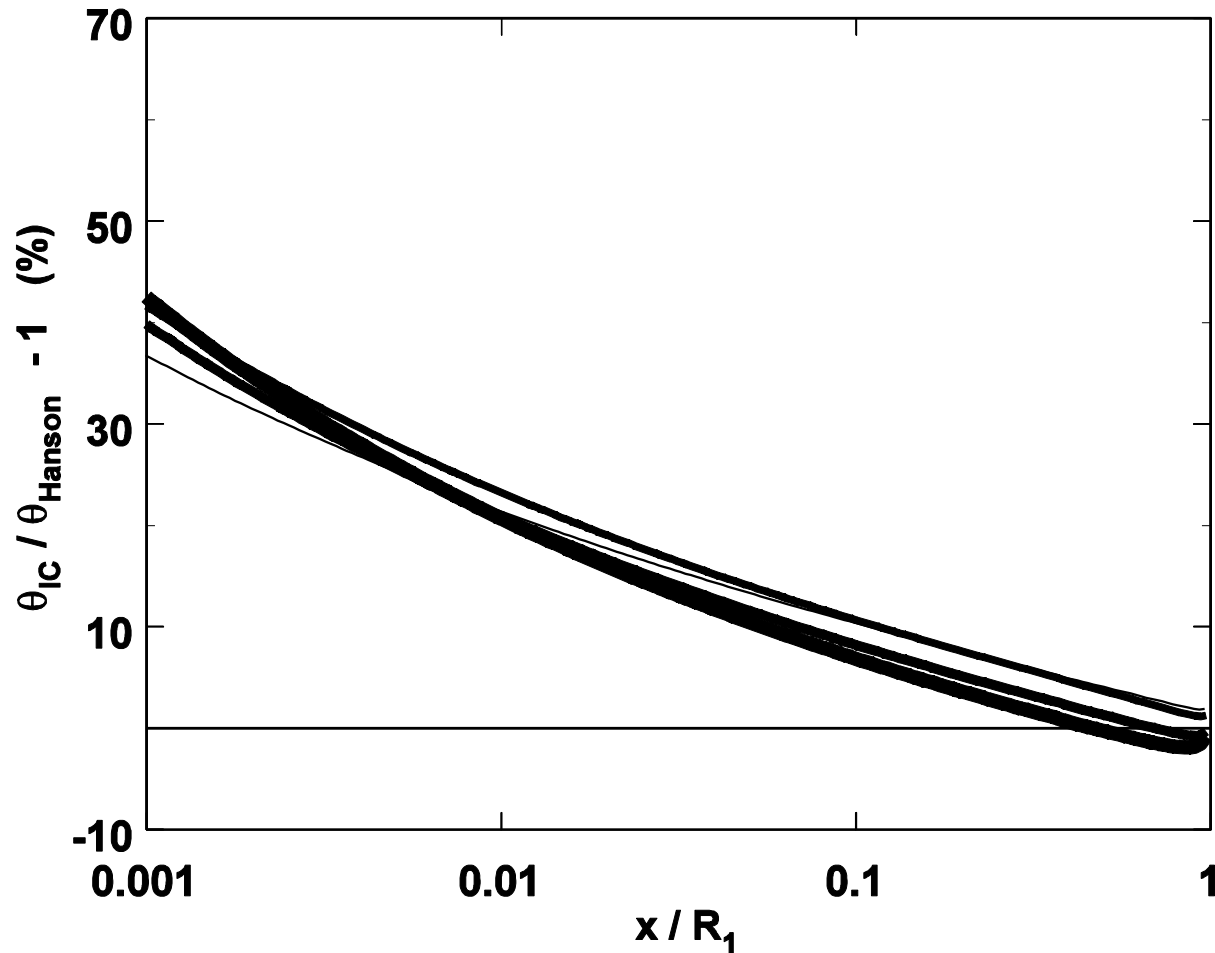
whereupon

$$T_{\text{IC}} = \left(\frac{E_s}{pv} \right)^2 \frac{1}{X_S}$$

identical in form and kinematic dependence to T_{FR} . The result is greatly improved material dependence but the same problem for thin targets.

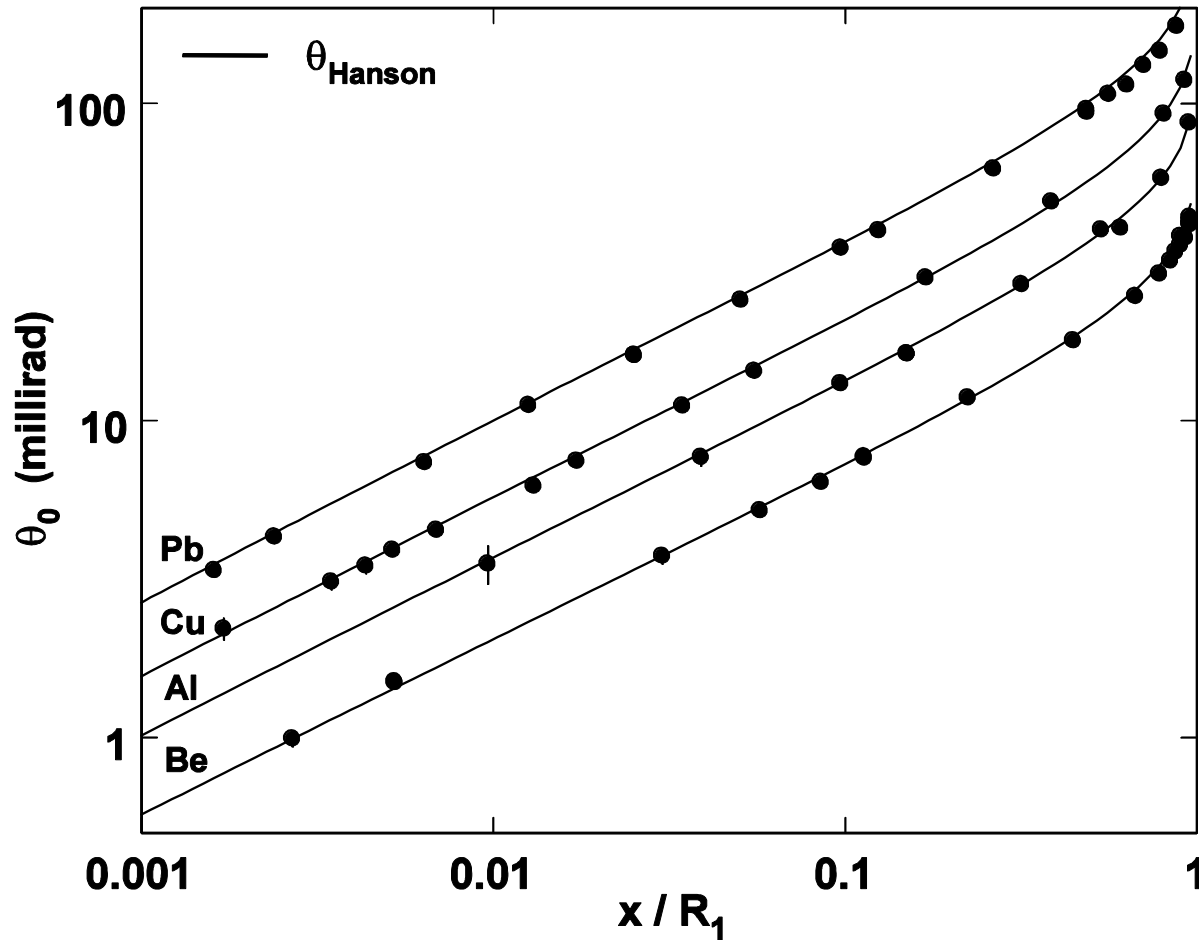


The 'ICRU Report 35' Scattering Power T_{IC}



For protons, T_{IC} is as simple as T_{FR} and considerably improved. We will use it as a building block, adding a single scattering correction (nonlocal term) to improve accuracy for thin scatterers.

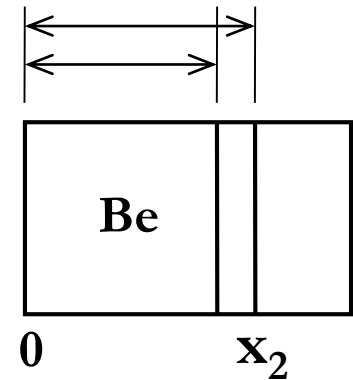
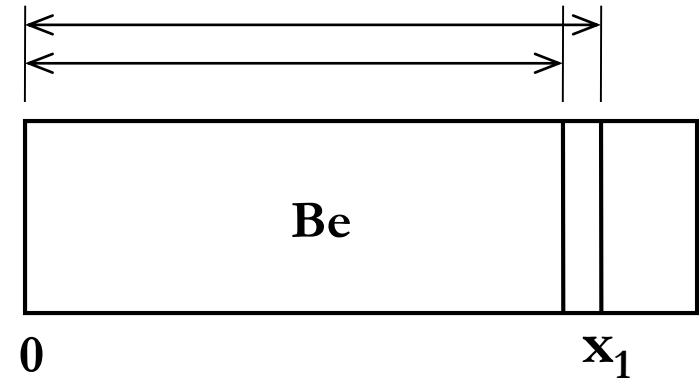
The Real Answer



Gottschalk et al. NIM **B74** (1993) 467-490. Molière/Fano/Hanson theory predicts θ_0 to a few percent over a wide range of target materials and normalized target thicknesses. We can use it to deduce the correct numerical value of T for any useful materials and thicknesses.

Finding the Real T

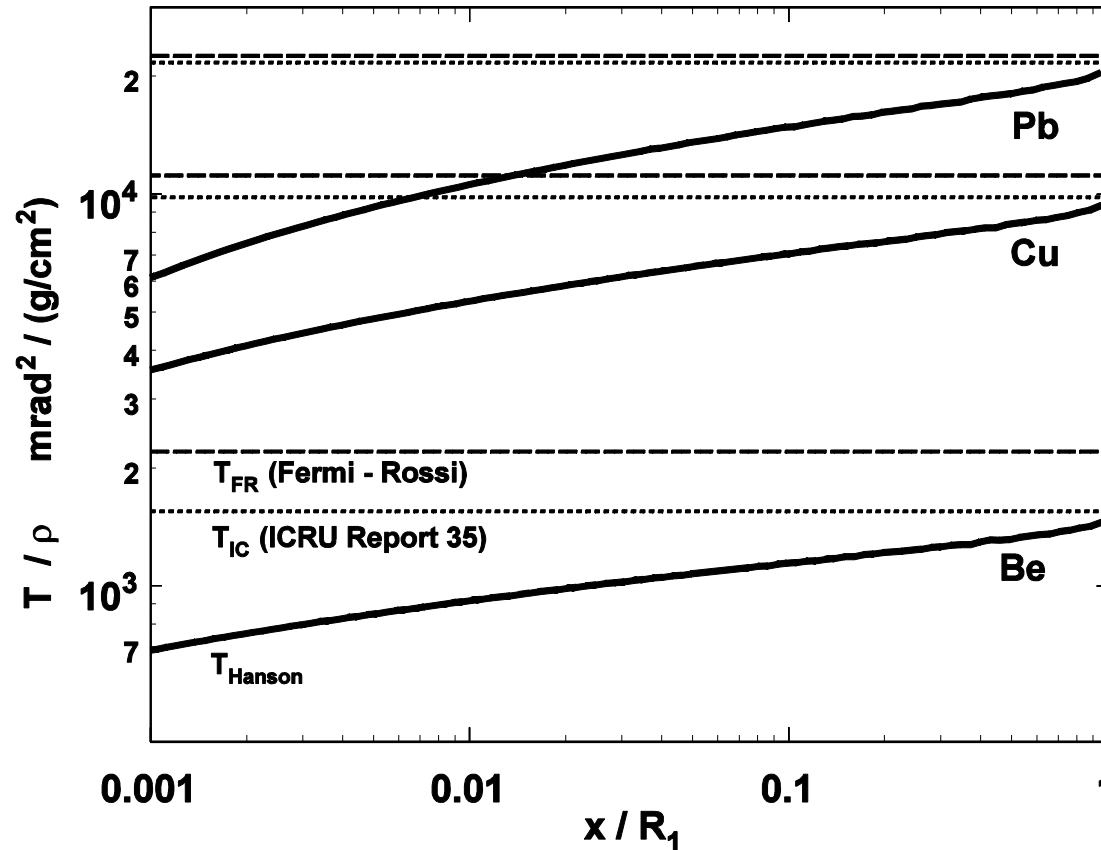
Suppose we want to find T in Be at 20 MeV. That question is not well posed, because a point where the proton has 20 MeV can have any amount of overlying material \mathbf{x} (cm). Two cases are shown at right. For any given case we can find the correct value of T by differentiating Molière/Fano/Hanson theory numerically (below). However, that involves a lengthy calculation and therefore does not directly yield a useful expression for T . We need to parameterize it somehow.



20 MeV

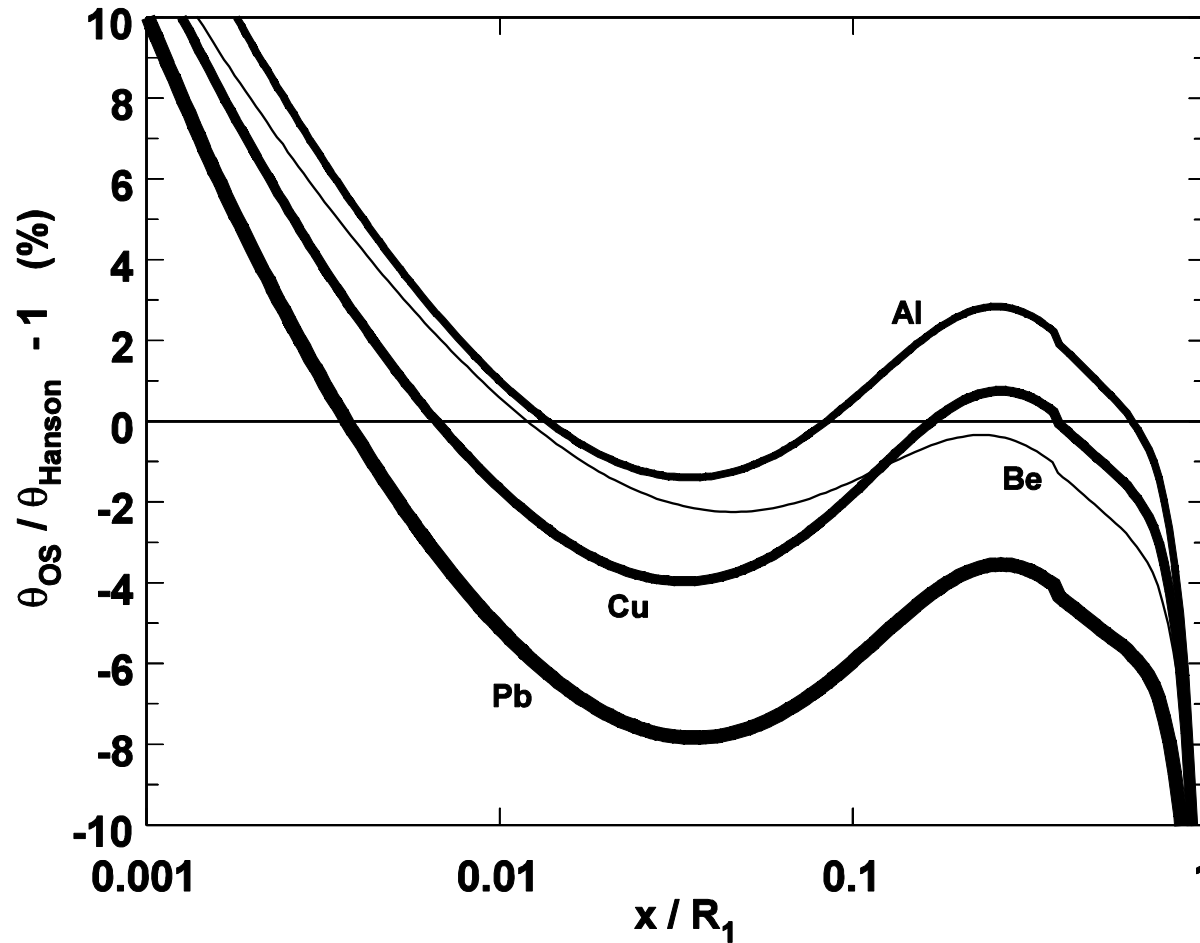
$$T_{\text{Hanson}}(\text{Be}, 20 \text{ MeV}, x) \equiv \frac{d\theta_{\text{Hanson}}^2}{dx} = \lim_{\Delta x \rightarrow 0} \frac{\theta_{\text{Hanson}}^2(x) - \theta_{\text{Hanson}}^2(x - \Delta x)}{\Delta x}$$

The Single Scattering Correction



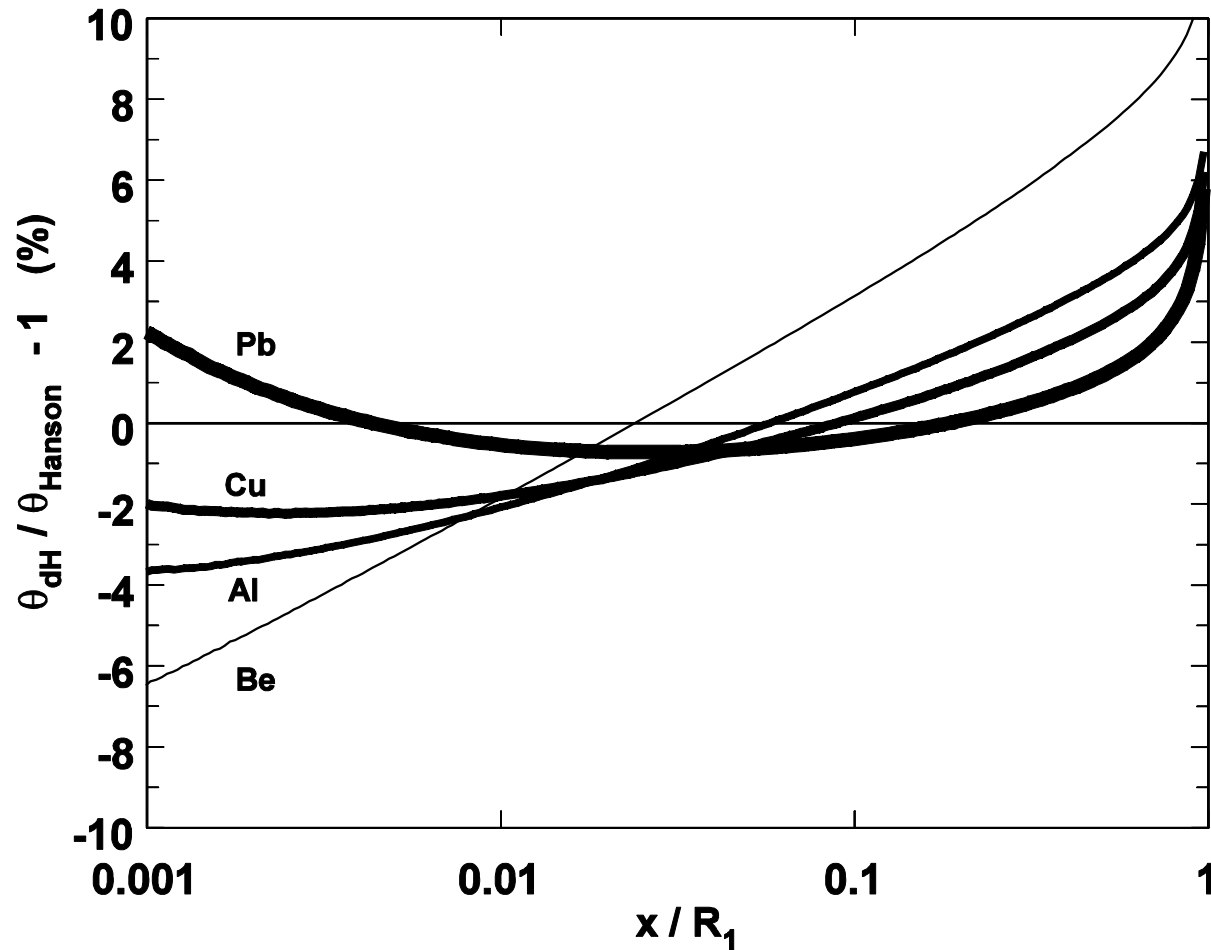
The result for 20 MeV protons in three materials, over a range of x 's (total thickness) relevant to proton therapy calculations. To improve the graph we have plotted *mass* scattering power vs. *normalized* thickness. T_{FR} and T_{IC} are *local*; they do not care about overlying material. T_{Hanson} is *nonlocal*. The single scattering correction is larger, the thinner the degrader. We will now express T_{Hanson} as T_{IC} times an approximate single scattering correction and call the result T_{dM} .

The Øverås-Schneider Scattering Power



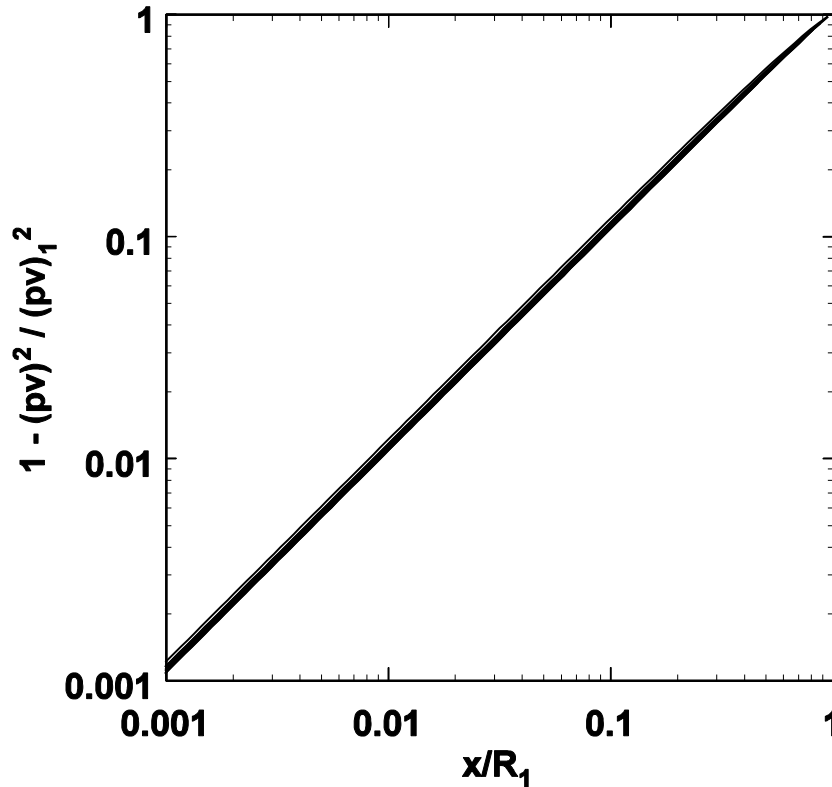
Schneider et al., Z. Med. Phys. **11** (2001) 110-118 propose a scattering power which is T_{FR} multiplied by a single scattering correction in the form of a polynomial in $t \equiv x/R_1$. For mixed slabs, regard t as that normalized depth which would result if the proton were degraded in the *current* material.

Kanematsu's Scattering Power T_{dH}



N. Kanematsu, NIM **B266** (2008) 5056-5062 describes a differential form of Highland's formula, obtained by multiplying T_{FR} by a single scattering correction factor which is logarithmic in a new pathlength integral l , the total x/X_0 traversed by the proton. This generalizes easily to mixed slabs.

The Øverås Approximation



$$(pv)^2 \approx (p_1 v_1)^2 (1 - x/R_1)$$

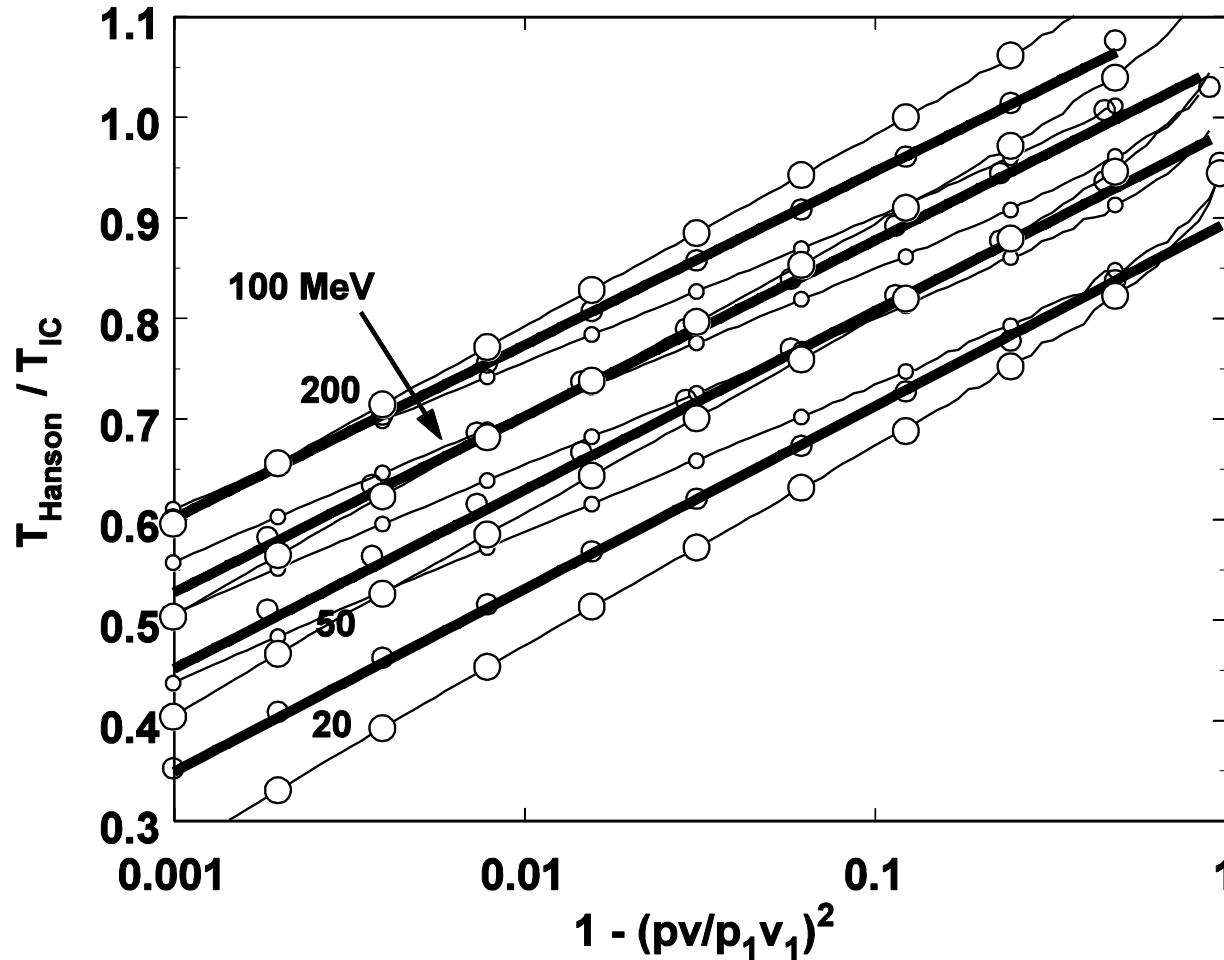
$$pv = \frac{\tau + 2}{\tau + 1} E$$

$$\tau \equiv \frac{E}{mc^2}$$

E \equiv kinetic energy

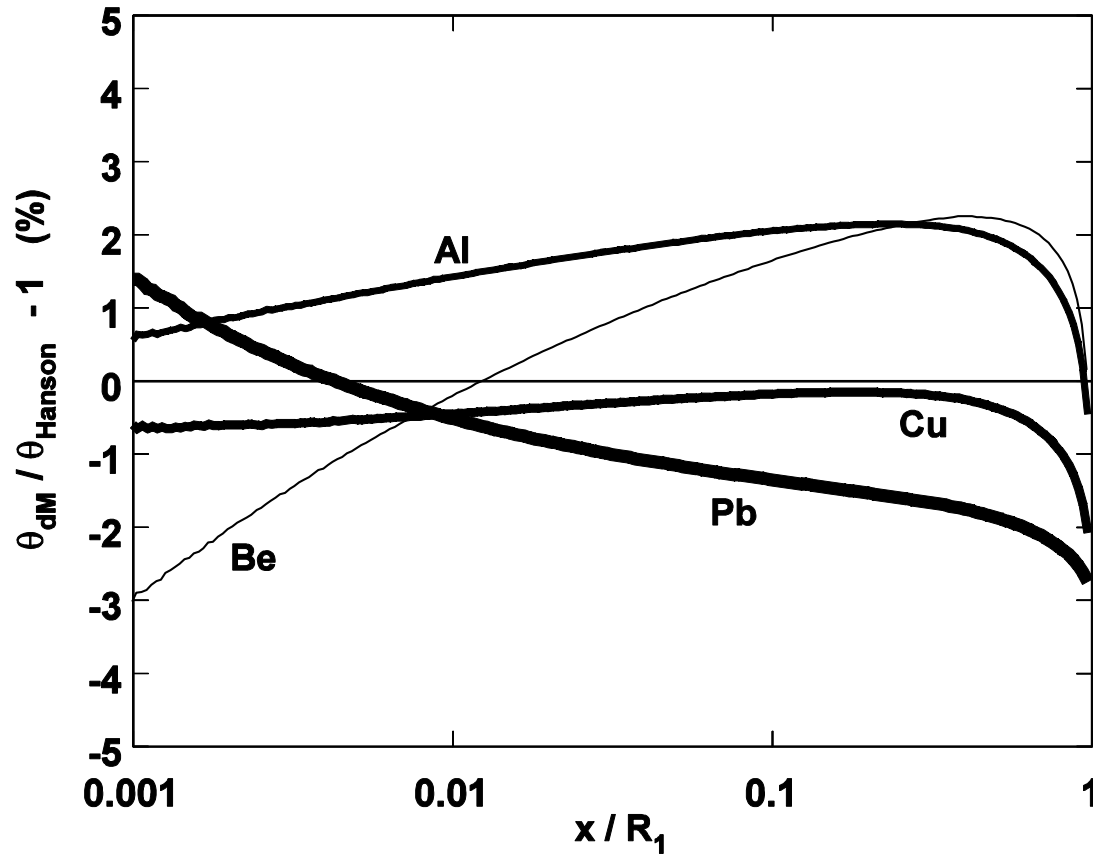
H. Øverås, CERN Yellow Report 60-18 (1960). If we express the single scattering correction directly as a function of x/R_1 it will not generalize gracefully to mixed slabs (different materials). The Øverås approximation lets us get around that.

The Single Scattering Correction Parameterized



Do the whole calculation for Be, Cu, and Pb, four local energies, and the whole interesting range of $\log_{10}(1 - (pv/p_1 v_1)^2)$. Plot $T_{\text{Hanson}}/T_{\text{IC}}$ and fit with a line whose coefficients are themselves linear in $\log_{10}(pv/\text{MeV})$.

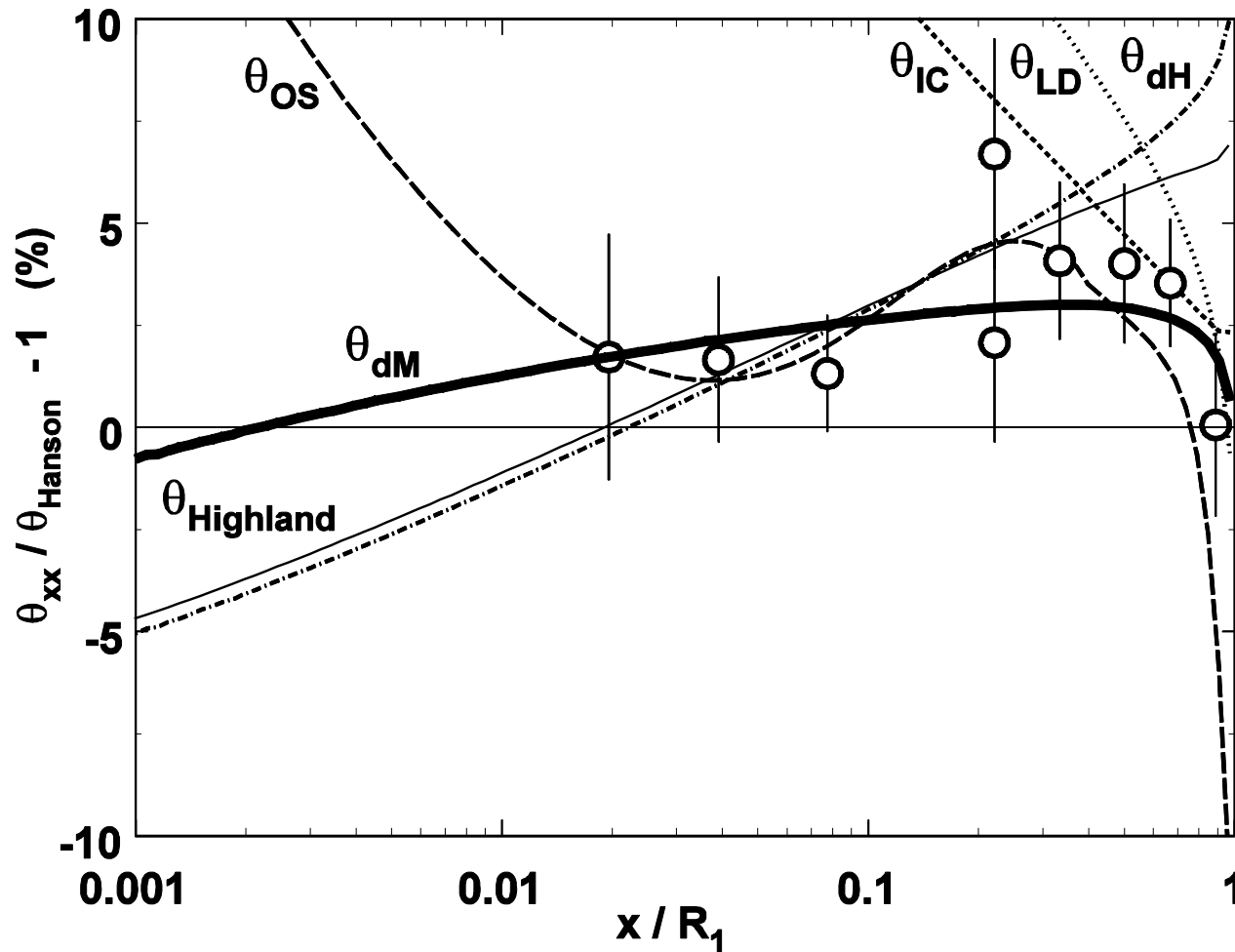
The Result: T_{dM}



$$T_{\text{dM}}(x) = f_{\text{dM}}(pv, p_1 v_1) \times \left(\frac{15.0 \text{ MeV}}{pv(x)} \right)^2 \frac{1}{L_S(x)}$$

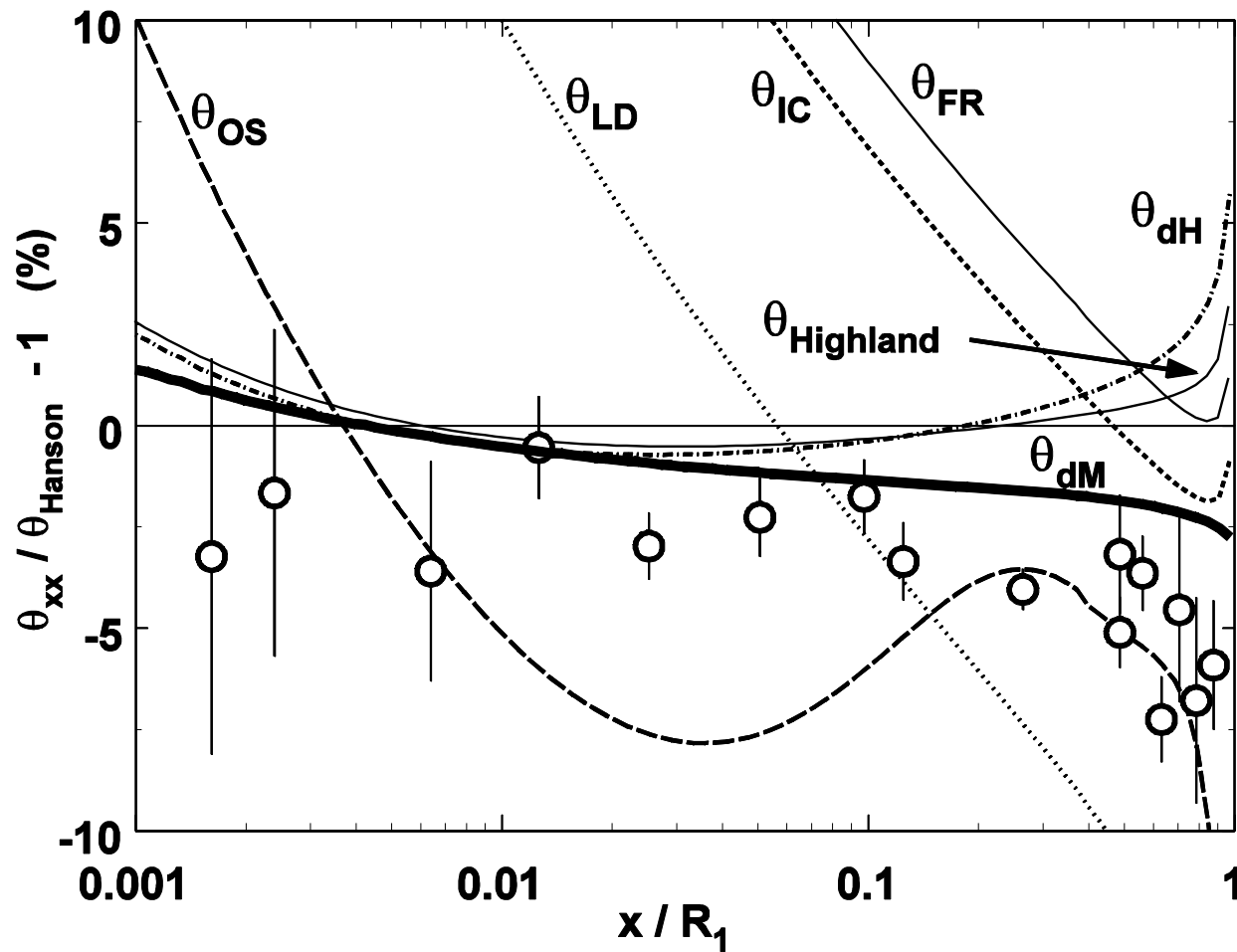
$$f_{\text{dM}} \equiv 0.5244 + 0.1975 \log_{10}(1 - (pv/p_1 v_1)^2) + 0.2320 \log_{10}(pv/\text{MeV}) \\ - 0.0098 \log_{10}(pv/\text{MeV}) \log_{10}(1 - (pv/p_1 v_1)^2)$$

Experimental Test, Polystyrene



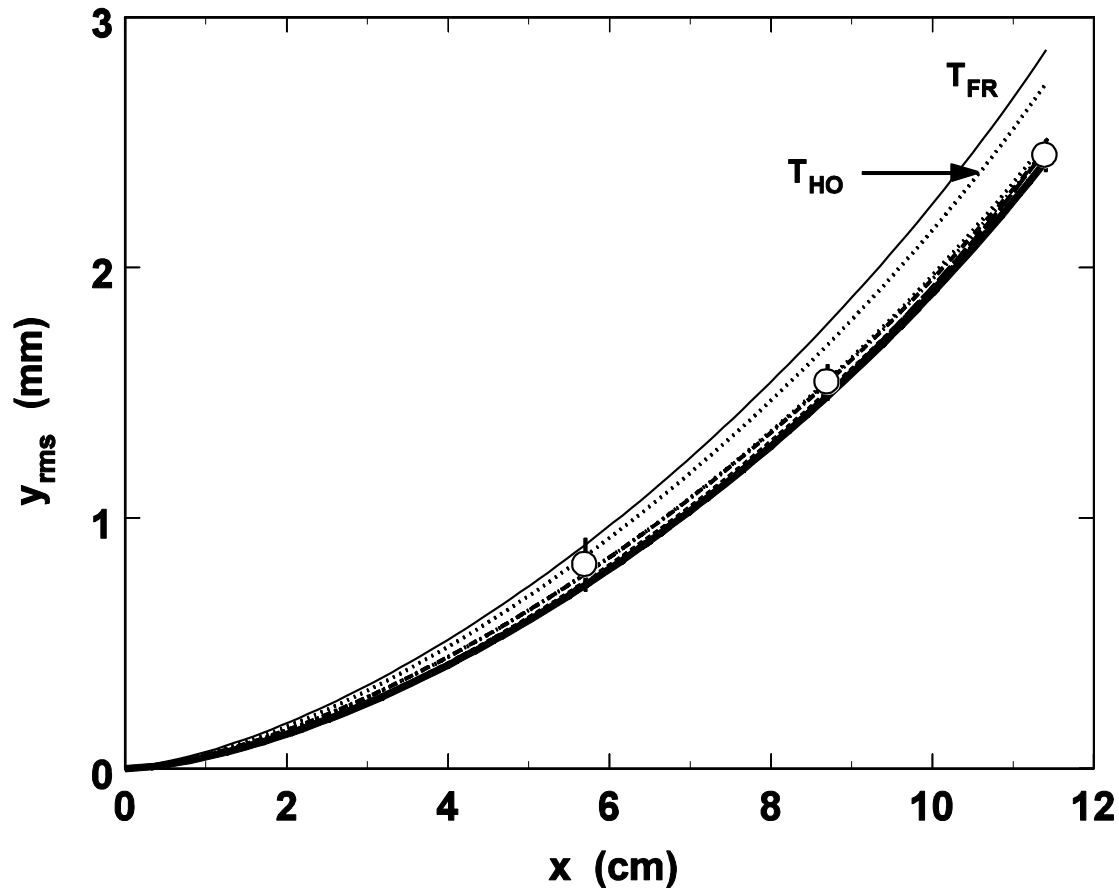
data/ θ_{Hanson} (Gottschalk et al. NIM B74 (1993) 467-490) along with results from all known formulas for T including another by Kanematsu ('corrected Rossi') and the generalized Highland formula Formulas for all are in the paper.

Experimental Test, Lead (Pb)



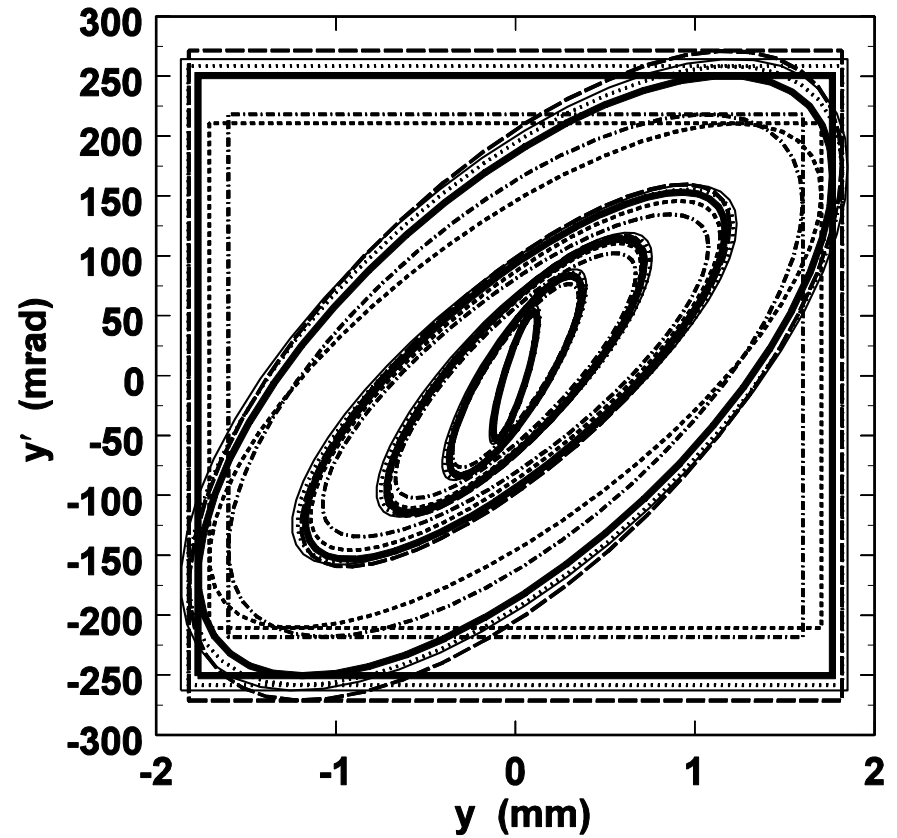
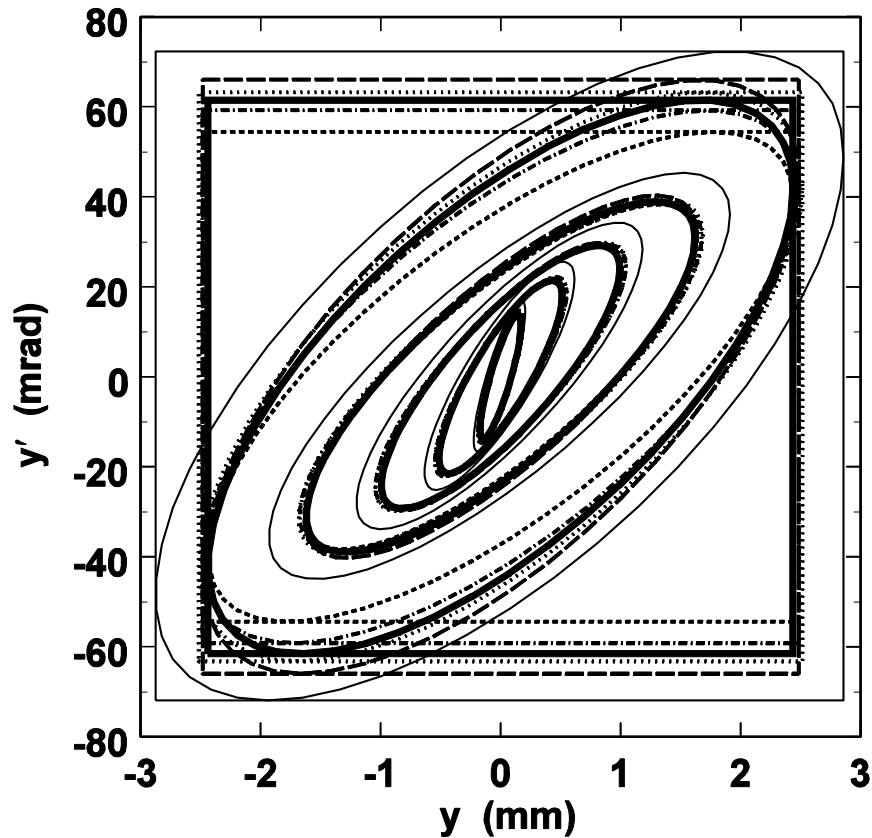
The same for Pb.

Does any of this matter ? Not in water.



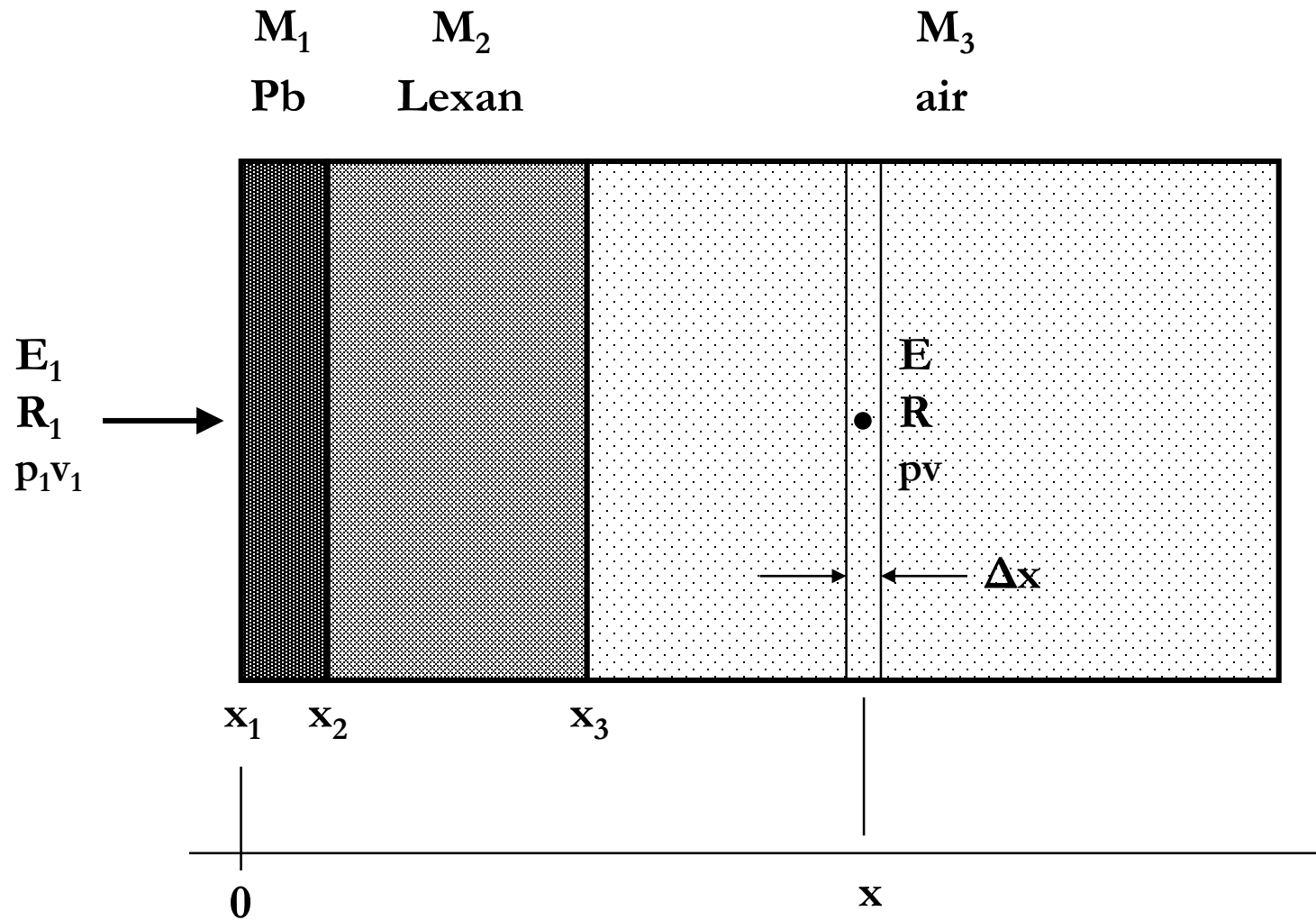
Except for T_{FR} and T_{HO} (which is simply wrong) beam spreading in light materials is remarkably insensitive to the formula for T . That is fortunate because it means that *dose reconstruction algorithms tend to be insensitive to T* . Thus, the ‘back end’ of a Monte Carlo simulation is insensitive to the MCS model.

Beam Spreading in H₂O and Pb



Evolution of Fermi-Eyges beam ellipses in near stopping targets of water (left) and Pb (right) for 127 MeV protons. Shows that the insensitivity of beam spreading to T is a fortuitous property of water-like materials. If we were computing slit scattering in brass or Cerrobend, T would make some difference.

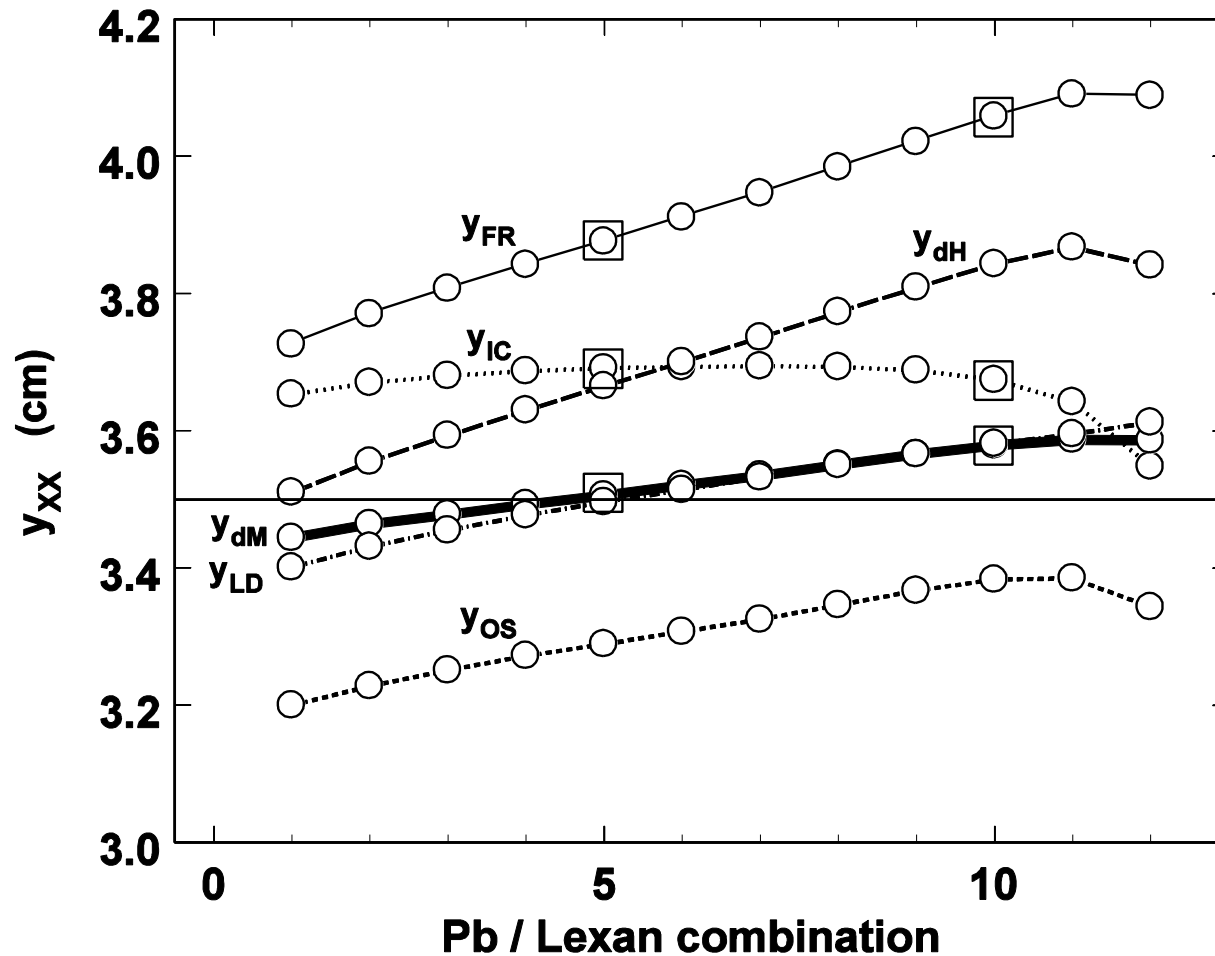
But suppose we have an upstream modulator ...



... as in the standard IBA proton nozzle.

comb #	Pb g/cm ²	Lexan g/cm ²	E_2 MeV	E_3 MeV	E_4 MeV	$\theta_{\text{Hanson}, 3}$ mrad	x_0 cm
1	6.429	0.000	216.4	216.4	215.9	35.10	0.28
2	6.173	2.560	216.9	206.4	205.9	35.12	0.34
3	5.872	5.144	217.6	196.1	195.6	35.19	0.53
4	5.543	7.743	218.3	185.4	184.9	35.32	0.88
5	5.179	10.360	219.1	174.3	173.8	35.51	1.44
6	4.781	12.995	219.9	162.7	162.2	35.79	2.23
7	4.335	15.656	220.9	150.5	150.0	36.19	3.30
8	3.834	18.346	221.9	137.5	137.0	36.73	4.71
9	3.240	21.085	223.2	123.7	123.1	37.45	6.55
10	2.509	23.898	224.7	108.6	108.0	38.42	8.94
11	1.537	26.840	226.8	91.8	91.1	39.78	12.11
12	0.000	30.082	72.2	72.2	71.5	41.93	16.54

Table 6: Pb/Lexan combinations of the simplified range modulator used in computing Figure 20. E_i is the proton energy entering the i^{th} slab ($E_1 = 230$ MeV), $\theta_{\text{Hanson}, 3}$ is the design MCS angle entering air and x_0 is the effective scattering point used in designing the modulator for constant $y_{rms} = 3.5$ cm at 100 cm. The pullback per position is 2.308 cm water equivalent.



Beam rms width at the exit of the Pb/Lexan/air stack (that is, at the second scatterer) for each step of the ‘modulator’ and for six scattering powers. If the actual width does not match the design width (3.5 cm) the dose at the patient will not be flat. Open squares are MC results, which agree with Fermi-Eyges. *The front end (beam line) of a proton MC calculation is sensitive to the MCS model !*

Answers

Scattering power (T) is a differential approximation to MCS theory.

We need it for charged particle transport, deterministic or Monte Carlo.

If we try to *start* with a differential form we get the wrong answer, especially for thin scatterers, because that assumes the Gaussian approximation is exact.

To improve simple (local) formulas for T we need a ‘single scattering correction’.

The correct theory of multiple Coulomb scattering in the Gaussian approximation is Molière/Fano/Hanson theory.

The correct numerical value of T can be obtained for any single slab problem by differentiating MFH theory numerically, but that is not useful by itself .

With the aid of the Øverås approximation T can be written in a simple form applicable to mixed slabs. The single scattering correction is expressed as a logarithmic function of current p_v and initial p_v . (An accurate T is necessarily non-local.)

In many problems, T (that is, the MCS model) makes no difference, but sometimes it does!