

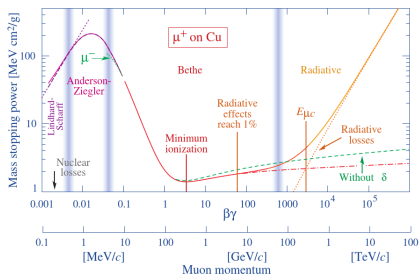
# Precise computation of the density effect correction

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University of Minnesota

12 July 2019

## Introduction



## PDG:

## 33.2.3. Stopping power at intermediate energies :

The mean rate of energy loss by moderately relativistic charged heavy particles is well-described by the “Bethe equation,”

$$\left\langle \frac{dE}{dx} \right\rangle = K z^2 \frac{Z}{A} \frac{1}{\beta^2} \left[ \frac{1}{2} \ln \frac{2m_e c^2 \beta^2 \gamma^2 W_{\max}}{I^2} - \beta^2 - \frac{\delta(\beta\gamma)}{2} \right]. \quad (33.5)$$

- “As the particle energy increases, its electric field flattens and extends, so that the distant-collision contribution to Eq. (33.5) increases as  $\ln \beta\gamma$ . However, real media become polarized, limiting the field extension...”
- Relevant for  $\beta\gamma \gtrsim 1$ 
  - i.e. kinetic energies: electrons  $\gtrsim 0.2$  MeV, muons 40 MeV, protons 400 MeV
- Tricky to compute for  $\beta\gamma \lesssim 8$ 
  - $\lesssim 30$  MeV (e), 700 MeV ( $\mu$ ), 6 GeV (p)
- At  $\beta\gamma \gtrsim 8$ ,  $\delta$  is well approximated by a simple form (such that “the mean excitation energy  $I$  is replaced by the plasma energy  $\hbar\omega_p$ .”)

## Sternheimer 1952

- R. M. Sternheimer. *The density effect for ionization loss in materials*. Phys. Rev., 88:851–859, 1952.
- Generalized Fermi's 1940 model to any number of oscillators
- Each "oscillator" is an atomic subshell, e.g. one for hydrogen and helium, three for carbon, etc.
  - Some ambiguities about conduction electrons, electrons in molecular orbitals, etc.

PHYSICAL REVIEW

VOLUME 88, NUMBER 4

NOVEMBER 15, 1952

### The Density Effect for the Ionization Loss in Various Materials\*

R. M. STERNHEIMER

*Brookhaven National Laboratory, Upton, New York*

(Received July 2, 1952)

The density effect for the ionization loss of charged particles has been calculated for a number of metals, scintillating materials, gases at various pressures, and photographic emulsion, using a dispersion model involving an appropriate number of dispersion oscillators for each substance. The results are presented in the form of graphs which can be used to correct the ionization loss for the density effect. The theoretical curves for silver chloride and anthracene are in reasonable agreement with experiments on the ionization loss of  $\mu$ -mesons. A general derivation of the equations for the density effect is given.

## Sternheimer 1984

- R. M. Sternheimer, M. J. Berger, and S. M. Seltzer.  
*Density effect for the ionization loss of charged particles in various substances.*  
Atom. Data Nucl. Data Tabl., 30:261, 1984.
- Refines treatment
  - Lorentz-Lorenz correction
  - Don't assume effect goes to zero in metals at low  $\beta\gamma$

### DENSITY EFFECT FOR THE IONIZATION LOSS OF CHARGED PARTICLES IN VARIOUS SUBSTANCES

R. M. STERNHEIMER

Department of Physics, Brookhaven National Laboratory  
Upton, New York 11973

and

M. J. BERGER and S. M. SELTZER

Center for Radiation Research  
National Bureau of Standards  
Washington, D. C. 20234

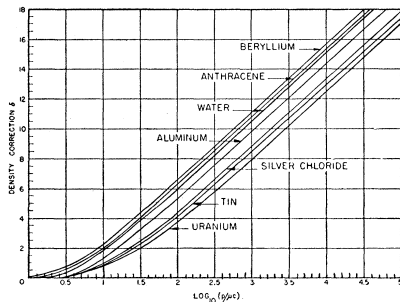
The density-effect correction  $\delta(\beta)$  for the ionization energy loss of charged particles has been evaluated as a function of the particle velocity for a total of 278 substances, including 98 cases of elements of the periodic table (12 gases and 86 condensed materials, including liquid hydrogen and graphite of three different densities) and 180 chemical compounds and substances of biological interest (13 gases and 167 liquid or solid substances). In the calculations, up-to-date values of the mean excitation potential  $I$  and of the atomic absorption edges  $h\nu_i$  were employed as input data for the general equations for  $\delta(\beta)$  previously derived by Sternheimer.

## Sternheimer method

- Sternheimer 1952 and 1984 give method for determining “exact” density effect
- I will call it “exact”, but it relies on several approximations, primarily:
  - Substances are made of isolated atoms with discrete energy levels
  - Only distant collisions contribute to  $dE/dx$
  - Effective oscillator frequencies are subshell energies scaled up to match mean ionization energy
- Computationally difficult without **electronic computers**
  - Have to solve (to good precision) a  $n$ -degree polynomial where  $n$  is the number of oscillators
- Inputs:
  - Mean ionization energy,  $I$
  - $\bar{\nu}_i$ : “oscillator frequency” = effective ionization energies (modulo  $h$ )
  - $f_i$ : “oscillator strength” = fraction of electrons with  $\bar{\nu}_i$
  - Obtain from tables (G4AtomicShells)

## Sternheimer approximation

- Because of difficulty of solving for  $\delta$ , Sternheimer 1952 provides an approximation:
  - Below some value  $\delta$  is zero
  - Then it's curved upwards as a function of  $\log(p)$
  - Then straight as a function of  $\log(p)$



In order to give more accurate values of  $\delta$ , which do not involve the use of Figs. 1 and 2, the calculated values of  $\delta$  have been fitted by means of an analytic expression as follows:

$$\delta = 4.606x + C + a(x_1 - x)^m, \quad (x_0 < x < x_1) \quad (10)$$

$$\delta = 4.606x + C, \quad (x > x_1) \quad (10a)$$

where  $x = \log_{10}(p/\mu c)$  and  $a$ ,  $m$ ,  $C$  are constants which depend on the substance;  $x_0$  is the value of  $x$  which corresponds to the momentum below which  $\delta = 0$  [see Eq. (9a)];  $x_1$  corresponds to the momentum above which the relation between  $\delta$  and  $x$  can be considered to be linear. The linearity of  $\delta$  at large energies can be seen from Figs. 1 and 2. The linear relationship is

- Values for  $m$ ,  $a$  and the cut-offs  $x_0$  and  $x_1$  are given for several substances
- Any reference to  $\{m, a, x_0, x_1, C\}$  means the approximation is in use

## Development of the approximation

- R. M. Sternheimer and R. F. Peierls.  
*General expression for the density effect for the ionization loss of charged particles.* Phys. Rev., B3:3681–3692, 1971.
- Confusingly, “general expression” means “further approximation”
  - Method for finding *rough* values of the  $\{m, a, x_0, x_1, C\}$  if computation to find *good* values for them hasn't been done
  - This is doubly approximate relative to the “exact” method
- Besides refining the exact method, Sternheimer 1984 also tabulates parameter values for the approximation for many substances
  - Geant4 uses these if a substance is tabulated, e.g. iron
  - Otherwise, “general expression” is used, no matter how similar it is to a tabulated material, e.g. steel (98% iron)

PHYSICAL REVIEW B

VOLUME 3, NUMBER 11

1 JUNE 1971

### General Expression for the Density Effect for the Ionization Loss of Charged Particles\*

R. M. Sternheimer and R. F. Peierls  
 Brookhaven National Laboratory, Upton, New York 11973  
 (Received 21 January 1971)

This paper presents a simple reformulation of the expression for the density effect correction  $\delta$ , i. e., the reduction in the ionization loss of fast charged particles due to the dielectric polarization of the medium. The general expression for  $\delta$  thus obtained is applicable to both condensed materials and gases. Its accuracy is such that the resulting values of the ionization loss  $dE/dx$  are expected to have a maximum error of less than 2% throughout the range of momenta where the density effect is important.

## Implementation of exact form in Geant4

- Not computationally difficult on a modern computer
- My patch has been submitted as **"Problem" 2121**
  - Patch is 813 lines
  - Lots of comments, some boilerplate: Only about 300 lines of new code



## Outline of implementation

- Implementation of Sternheimer 1984, § “Numerical Evaluation of the Density Effect”
  - Ignoring the following sections, “Fitting Formula”, etc., which are about approximation

### Numerical Evaluation of the Density Effect

The calculations of  $M(\beta)$  are based on the following equations, derived by Sternheimer<sup>3,2</sup> in 1945 and 1952:

$$M(\beta) = \sum_{\rho=1}^n f_{\rho} \ln [(l_{\rho}^2 + l^2)/l_{\rho}^2] - l^2(1 - \beta^2), \quad (1)$$

where  $\beta = v/c$  is the particle velocity divided by the velocity of light, and  $l$  is the solution of the equation,

$$\frac{1}{\beta^2} - 1 = \sum_{\rho=1}^n \frac{f_{\rho}}{\bar{v}_{\rho}^2 + l^2}, \quad (2)$$

where  $n$  is the number of dispersion oscillators required to describe the atoms of the medium and the  $f_{\rho}$  are the corresponding oscillator strengths. In Eq. (2),  $\bar{v}_{\rho}$  is defined by

$$\bar{v}_{\rho} = v_{\rho}/v_p, \quad (3)$$

where  $h\nu_{\rho}$  is the absorption edge for the  $\rho$ th oscillator of the dispersion model. The quantity  $h\nu_p$  is the plasma energy of the electrons of the substance considered as free electrons, and is given by<sup>2</sup>

$$h\nu_p = 28.816(\rho_0 Z/A)^{1/2} \text{ eV}, \quad (4)$$

where  $\rho_0$  is the density of the medium (in g/cm<sup>3</sup>),  $Z$  is the atomic number, and  $A$  is the atomic weight. In the case of a compound or molecular gas,  $Z/A$  is to be replaced

by the ratio of the total number of electrons to the effective molecular weight or the sum of atomic weights of the constituent atoms:  $\Sigma Z_i/\Sigma A_i$ . As in Ref. 12, a separate dispersion oscillator is used for each subshell of the atom considered, e.g., K, L<sub>1</sub>, L<sub>2,3</sub>, and L<sub>III</sub> for neon. The quantity  $\rho$  in Eq. (3) is the adjustment factor which was introduced by Sternheimer<sup>3</sup> in 1952 and which is designed to give agreement of the oscillator energies  $h\nu_{\rho}$  (or rather  $h\nu_{\rho}/\rho$ ) with the observed mean excitation potential  $I$ . Specifically, in Eq. (1), the constants  $l_{\rho}$  are defined by

$$l_{\rho} = [v_{\rho}^2 + (2/3)f_{\rho}]^{1/2} \quad \text{for } \bar{v}_{\rho} > 0 \quad (5)$$

$$l_{\rho} = f_{\rho}^{1/2} \quad \text{for } \bar{v}_{\rho} = 0 \quad (6)$$

(for conduction electrons in a metal).

In Eq. (5), the factor 2/3 takes into account the Lorentz-Lorenz correction [see Ref. 5, Eqs. (48)–(52)] in the expression for the polarizability  $\alpha(\nu)$ ; note that this factor does not enter for the case of conduction electrons for which  $l_{\rho} = f_{\rho}^{1/2}$ , as given above.

The mean excitation potential  $I$  of the medium is given by

$$\ln I = \sum_{\rho} f_{\rho} \ln (h\nu_{\rho}). \quad (7)$$

By making use of Eq. (3) for  $\bar{v}_{\rho}$ , we obtain the following expression, which is used to determine the value of the Sternheimer adjustment factor  $\rho$ :

$$\ln I = \sum_{\rho=1}^{n-1} f_{\rho} \ln [(h\nu_{\rho})^2 + (2/3)f_{\rho}(h\nu_{\rho})^2]^{1/2} + f_n \ln (h\nu_p f_n^{1/2}). \quad (8)$$

- User specifies if material is a **conductor**:  
`GetMaterialPropertiesTable()`  
`->AddConstProperty("conductor", 1)`
  - Materials are insulators by default
- First, solve Eq. (8) to find scaling factor  $\rho$  in `SetupFermiDeltaCalc()`
  - Numeric, Newton's method
    - Evaluated once during initialization, no heavy lift per step
- Uses tabulated mean ionization energy,  $I$
- Can have no solution if user gives very high density for which  $I$ -value is invalid
  - e.g. hydrogen at 10 g/cc
  - Print detailed warning, fall back to approximation
  - Approximation won't be good either!

## Outline of implementation, continued

### Numerical Evaluation of the Density Effect

The calculations of  $\delta(\beta)$  are based on the following equations, derived by Sternheimer<sup>3,5</sup> in 1945 and 1952:

$$\delta(\beta) = \sum_{i=1}^n f_i \ln [(l_i^2 + l^2)/l_i^2] - l^2(1 - \beta^2), \quad (1)$$

where  $\beta = v/c$  is the particle velocity divided by the velocity of light, and  $l$  is the solution of the equation,

$$\frac{1}{\beta^2} - 1 = \sum_{i=1}^n \frac{f_i}{\tilde{\nu}_i^2 + l^2}, \quad (2)$$

where  $n$  is the number of dispersion oscillators required to describe the atoms of the medium and the  $f_i$  are the corresponding oscillator strengths. In Eq. (2),  $\tilde{\nu}_i$  is defined by

$$\tilde{\nu}_i = \nu_{i0}/\nu_p, \quad (3)$$

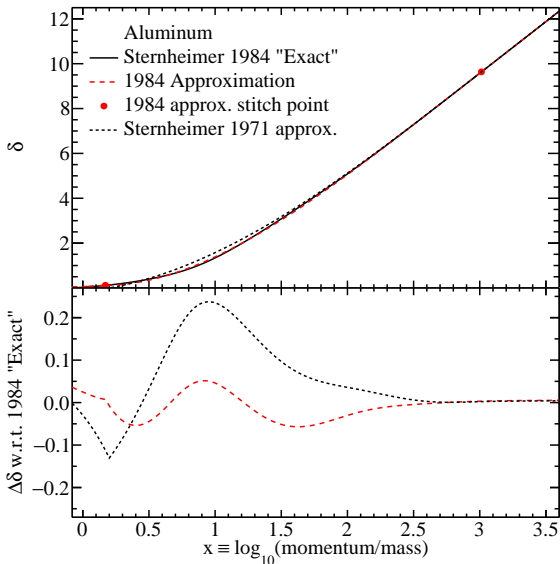
where  $\nu_{i0}$  is the absorption edge for the  $i$ th oscillator of the dispersion model. The quantity  $h\nu_p$  is the plasma energy of the electrons of the substance considered as free electrons, and is given by<sup>20</sup>

$$h\nu_p = 28.816(\rho_0 Z/A)^{1/2} \text{ eV}, \quad (4)$$

where  $\rho_0$  is the density of the medium (in  $\text{g/cm}^3$ ),  $Z$  is the atomic number, and  $A$  is the atomic weight. In the case of a compound or molecular gas,  $Z/A$  is to be replaced

- Using  $\rho$ , solve Eq. (2) to find  $l$ , again with Newton's method
  - Evaluated once per energy bin in *Range* table, no heavy lift per step
  - Possible, in principle, for this to fail, but I haven't seen it
  - Print warning and fall back to approximation if it does
- With  $l$  in hand, evaluate Eq. (1) to find  $\delta$
- Check value of  $\delta$  against that gotten from the parameterized approximation
  - If they differ by more than 1.0, print warning and use approximation
  - However, if approximation is *negative* (unphysical), always use exact form. Can happen for substances with extremely low density, e.g. NOVA's "vacuum" with  $10^{-25}$  g/cc.
  - I have not found a case where this fall back is used

## Example: Aluminum

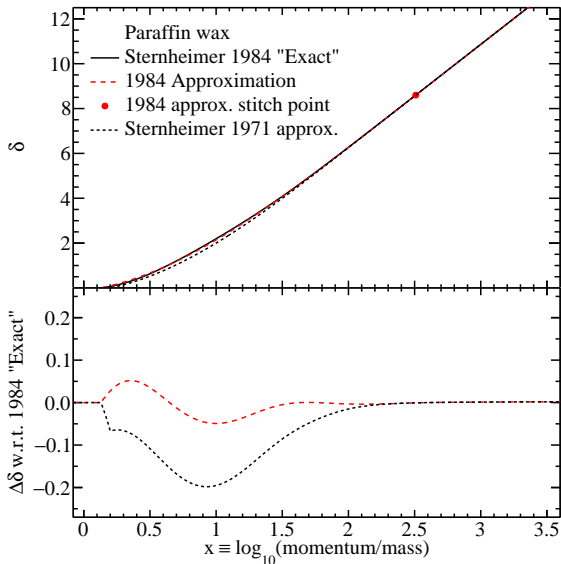


- Shows difference between results for exact form and tabulated approximation
- And between exact form and "general expression" (e.g. 99.99% aluminum)

In terms of  $dE/dx$ :

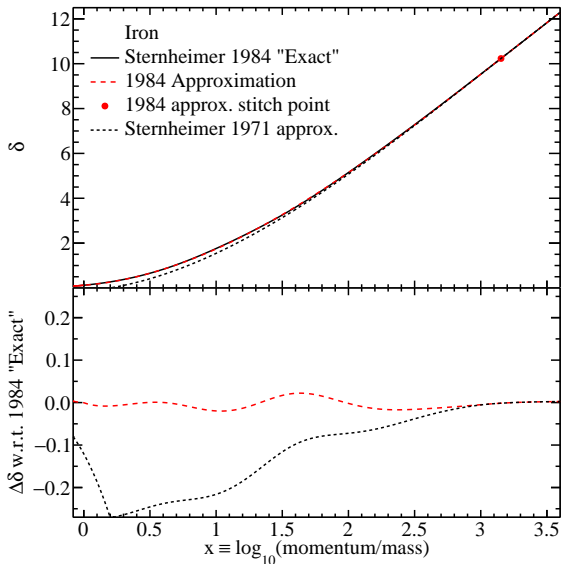
- $\delta$  contributes via  $K z^2 \frac{Z}{A} \frac{1}{\beta^2} \frac{\delta}{2}$
- Typically, 1 unit of  $\delta$  translates to  $\sim 0.07 \text{ MeV/g cm}^2$ , or  $\sim 5\%$
- Pure Al, exact form is 0.3% improvement (at max deviation)
- Impure Al, exact form is 1.1% improvement

## Example: paraffin wax



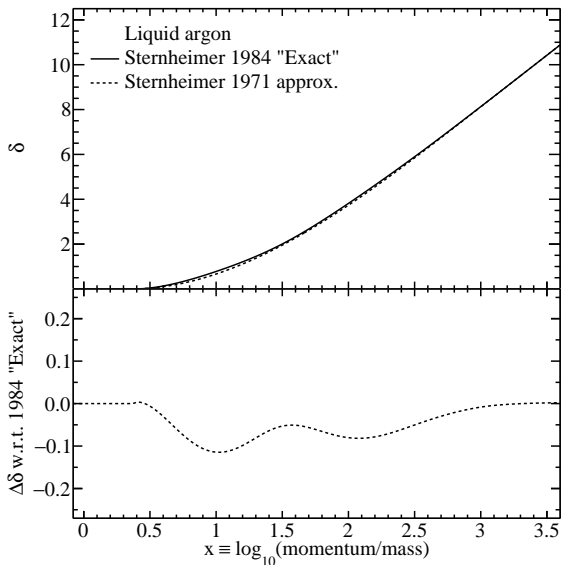
- Exact form is 0.3% improvement for exactly paraffin wax
- 1.0% improvement for similar hydrocarbons

## Example: iron



- Pure iron: 1984 approximation is quite close to the exact solution
- Impure iron (say, steel): 1971 approximation, up to 1.3% off

## Example: liquid argon



- Liquid argon is **not tabulated** by Sternheimer 1984
- Up to  $\sim 0.6\%$  deviation in  $dE/dx$  from 1971 double-approximation
- Notice how the density effect doesn't set in until  $x = 0.5$  (250 MeV for muons)
- That's because argon doesn't have any weakly bound electrons

## Dielectric response

- Using this Sternheimer “exact” form is certainly an improvement
- But is it close enough to **physical truth** for the difference to matter?
- ICRU 37: the “*most accurate method of evaluating the density-effect correction is to use semi-empirical dielectric-response functions*”, but “*Reliable and complete [ones ...] are scarce*”
- With dielectric-response functions, don't have to assume isolated atoms, no sharp insulator/conductor divide, etc.
- As far as I know, data is only available for water, aluminum and silicon

RADIATION RESEARCH **89**, 32-37 (1982)

## Density Effect in Liquid Water<sup>1,2</sup>

J. C. ASHLEY

*Health and Safety Research Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830*

ASHLEY, J. C. Density Effect in Liquid Water. *Radiat. Res.* **89**, 32-37 (1982).

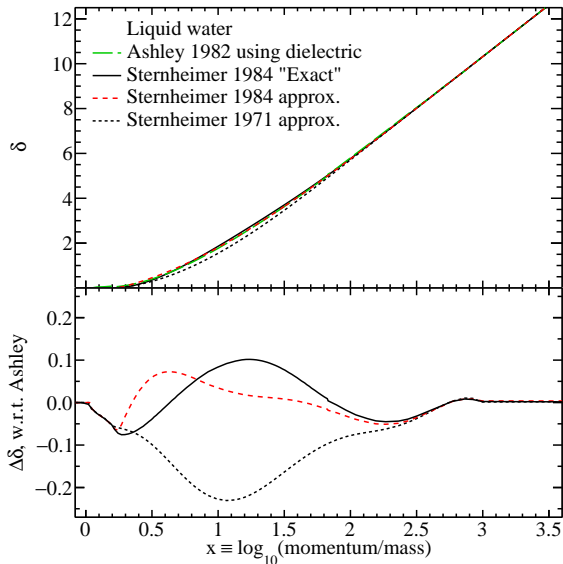
The density effect  $\delta$  in the stopping power of liquid water is evaluated. A model calculation for the imaginary part of the dielectric function is employed which is based in part on the limited optical data for water and on generalized oscillator strengths for ionization of the *K* shell of oxygen. Excellent agreement is found with Sternheimer's predictions for  $\delta$  at higher energies where  $\delta$  contributes significantly to the stopping power; large differences are found just above the threshold for the density effect but are at energies where  $\delta$  forms a relatively insignificant part of the stopping power. The largest deviation in the predicted stopping powers of water for electrons using the different results for  $\delta$  is  $\sim 1\%$  at  $\sim 5$ -6 MeV.

- Using "limited data" on  $\epsilon(iy)$  available for water, evaluated **more exact** form:

$$\delta = \frac{2}{\omega_p^2} \int_0^l [1 - 1/\epsilon(iy)] y dy - (l/\omega_p)^2 (1 - \beta^2)$$



## Example: Water



- Compared to **dielectric treatment**, Sternheimer "exact" is off by up to  $\sim 0.5\%$ 
  - $\pm 0.2\%$  from digitizing an old plot
- Sternheimer tabulated approximation also  $\sim 0.5\%$
- 1971 "general expression" (used for impure water)  $\sim 1.0\%$

## Comparison to dielectric treatment for aluminum, silicon

- Similar effort for aluminum, with better data and better plots:

PHYSICAL REVIEW B

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1 JANUARY 1982

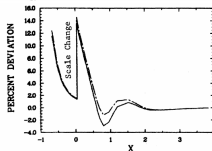
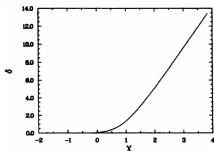
### Fermi density effect on the stopping power of metallic aluminum

Mitio Inokuti and David Y. Smith

*Argonne National Laboratory, Argonne, Illinois 60439*

(Received 2 July 1981)

The density-effect correction  $\delta$  to the Bethe stopping-power formula for fast charged particles is evaluated for metallic aluminum from the dielectric-response function  $\epsilon(E)$ . The latter has been accurately determined over the entire range of excitation energy  $E$  by Shiles, Sasaki, Inokuti, and Smith through comprehensive analysis of all pertinent experimental data. The resulting values of  $\delta$  (which is a function of the particle speed  $\beta c$ ) should be the most reliable to date. The present result agrees well with that of Sternheimer, who used a simpler and less rigorous procedure, and thus corroborates the general view that  $\delta$  is insensitive to fine details of the behavior of  $\epsilon(E)$ . We also present general remarks on the evaluation of  $\delta$  and on the analytic continuation of  $\epsilon(E)$  as a function of the complex energy  $E$ .



- Max deviation in  $\delta$  between Sternheimer "exact", dielectric: 0.03 (0.15% in  $dE/dx$ )
  - Max deviation between Sternheimer "exact" and tabulated approximation is 0.061
  - And from tabulated approximation to "general expression", 0.2
- Silicon: Bichsel, Rev.Mod.Phys. **60**, 663 (1998): max deviation 0.06 (0.3% in  $dE/dx$ )
  - Between Sternheimer "exact", tabulated approximation: 0.059

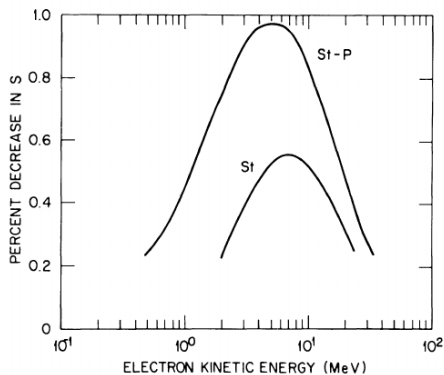
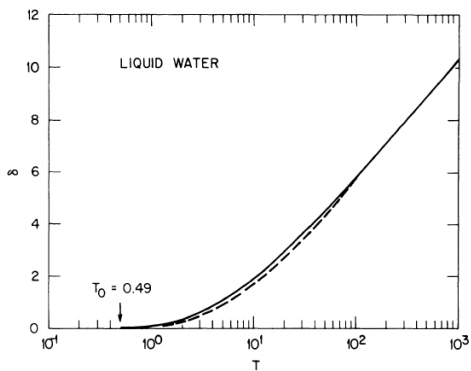
## Conclusions

- This patch implements the calculation from which the parameterized approximation Geant4 has been using derives
- **Confident that moving from Sternheimer “general expression” to exact form is an improvement**
  - This is what the patch does for most materials
- Moving from approximation with 1984 tabulated parameters to exact form is certainly an improvement, but may or may not be significant
  - Only relevant to pure elements, a few selected compounds and mixtures
- Avoids sudden change in behavior when user switches a tabulated material for a nearly-identical untabulated one
- No significant change to CPU usage
- Patch already used by NOvA to obtain improved  $dE/dx$  in steel by up to 1.3%
  - Important because this difference cannot be calibrated out in a neutrino experiment
  - Same will be true for DUNE at the level of 0.6%

# Backups

## More detail on Ashley 1982

Had to digitize plots for this, and the two plots in Ashley disagreed by up to 0.05



## Other Approximations

The  $\bar{\nu}_i$  must be obtained for each case from the energy levels of the atoms considered. As a first approximation, the frequencies are given by the ionization potentials  $h\nu_i$  of the  $K, L, M, \dots$  shells and the  $f_i$  are equal to the corresponding occupation numbers divided by the atomic number  $Z$ . The ionization potentials were obtained from the table given by Sommerfeld.<sup>8</sup> For the outermost shell, the tables of Bacher and Goudsmit<sup>9</sup> were also used. With the  $\nu_i$  thus obtained, the geometrical mean  $\nu_m$  of the frequencies is calculated; we have

$$\ln \nu_m = \sum_i f_i \ln \nu_i. \quad (4)$$

<sup>8</sup> A. Sommerfeld, *Atomic Structure and Spectral Lines* (Methuen and Company, London, 1934), third edition, p. 237.

<sup>9</sup> R. F. Bacher and S. Goudsmit, *Atomic Energy States* (McGraw-Hill Book Company, Inc., New York, 1932).

- Later amended to subshells, but that's still an approximation: atoms are not isolated

### SOMMERFELD

=principal quantum number). The  $f_i$  are  $2/47, 8/47, 18/47, 18/47, 1/47$ . The resulting  $h\nu_m$  is 25.2 ry, which is a factor 1.25 lower than the experimental value<sup>11</sup> of 31.5 ry. To obtain the frequencies to be used in Eq. (1) the  $\nu_i$  obtained from the ionization potentials were raised by the factor 1.25. This procedure was carried out for each substance. In the following, the experimental mean frequency is denoted by  $\nu_m'$  and the corrected transition frequencies are denoted by  $\nu_i'$ , so that

$$\nu_i' = (\nu_m' / \nu_m) \nu_i. \quad (7)$$

The factor  $\nu_m' / \nu_m$  is perhaps an indication that the average of the states to which the electrons are excited lies in the continuum above the ionization limit. The values of  $\bar{\nu}_i$  used in Eq. (1) are obtained from

$$\bar{\nu}_i = \nu_i' / \nu_p. \quad (8)$$

- Assumption that it makes sense to scale them all up uniformly
- Totally *ad hoc* as far as I know

## Other Approximations

### III. EQUATIONS FOR THE DENSITY EFFECT

In this section we give the derivation of the equations of the density effect which has been previously obtained.<sup>8</sup> If the electric field  $\mathbf{E}$  of the passing particle and the polarization  $\mathbf{P}$  of the medium are Fourier analyzed, a relation

$$\alpha(\omega)\mathbf{E}_\omega = 4\pi\mathbf{P}_\omega \quad (18)$$

is assumed to hold for the Fourier components of frequency  $\omega$ .  $\alpha(\omega)$  is  $4\pi$  times the polarizability, for which we write

$$\alpha(\omega) = \frac{4\pi n^2 e^2}{m} \sum_i i \frac{f_i}{\omega_i^2 - 2i\eta_i\omega - \omega^2} \quad (19)$$

where the atomic frequencies  $\omega_i$ , the damping constants  $2\eta_i$ , and  $\omega$  are to be expressed in rad/sec. It was shown by Fermi<sup>9</sup> that the ionization loss to atoms with impact parameter greater than  $b$  is given by

$$W_b = \frac{2e^2 b}{\pi v^3} \text{Rl} \int_0^\infty \left( \frac{1}{1+\alpha} - \beta^2 \right) i\omega k^* K_1(k^* b) K_0(kb) d\omega, \quad (20)$$

where  $K_0$  and  $K_1$  are the modified Bessel functions of the second kind, Rl denotes the real part, and  $k$  is the square root with real part  $\geq 0$  of

$$k^2 = \frac{\omega^2}{v^2} (1 - \beta^2) - \frac{\omega^2 \alpha}{c^2}. \quad (20a)$$

Upon using the approximate expressions for  $K_0$  and  $K_1$ ,

$$K_0(kb) \approx \frac{1}{2} \ln(4/3.17k^2 b^2), \quad (21)$$

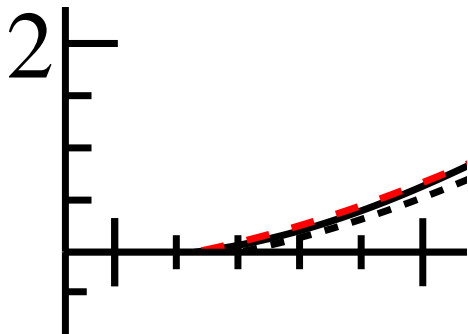
$$K_1(k^* b) \approx 1/k^* b, \quad (21a)$$

one obtains from Eq. (20)

$$W_b = \frac{4ne^4}{mv^2} \text{Rl} \int_0^\infty \left( 1 - \beta^2 - \frac{\alpha}{1+\alpha} \right) \left[ \ln \frac{4mv^2}{3.17\pi b^2 n^2 (1-\beta^2)} - 2 \ln v - \ln \left( 1 - \frac{\beta^2 \alpha}{1-\beta^2} \right) \right] i v d\nu, \quad (22)$$

- No treatment of the case when the ionization is at a small impact parameter
  - Minority of interactions
  - $\sim$ No screening when particle passes through atom being ionized?
  - Not sure what the size of this approximation is
- Don't know what the effect of the Bessel function approximation is

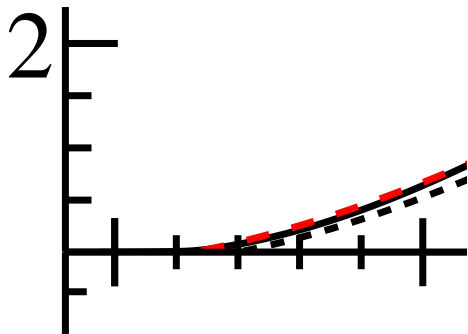
## Back to Paraffin Wax... "Exact"



- For non-conductors, "exact" form *and* approximations crash land at  $\delta = 0$
- I think this is **mostly because the theory treats all electrons as being bound in free atoms**
  - Paraffin: four classes with energies  $\{11.26, 16.59, 288\}$  eV (C) and 13.6 eV (H)
- Really there are a large number of more weakly bound molecular states, and some electrons in the conduction band (at finite temperature(?))
  - Applies to anything except an arbitrarily rarefied gas, for which  $\delta = 0$  anyway

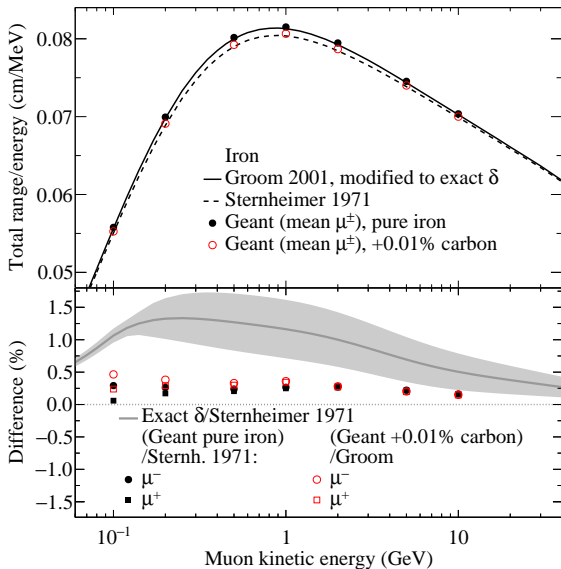


## "Exact"



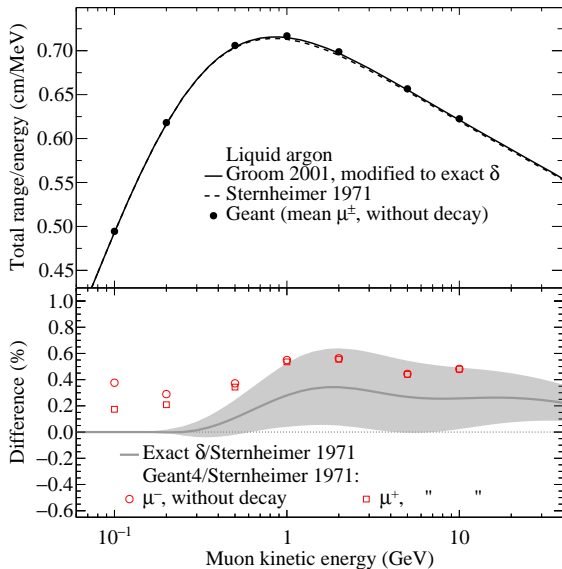
- If I move 0.5 of an electron to a zero-energy conducting band,  $\delta$  stays positive down to  $p/m \approx 10^{-6}$  (but then still breaks down there)

## Effect on muon range in NOvA Muon Catcher



- Get 1971 approximation for impure iron (steel-like)
- Get 1984 approximation for pure iron
- Geant4 is  $\sim 0.3\%$  high of Groom (another evaluation of 1984 approximation) for unknown reasons
  - 1.0% off the best estimate

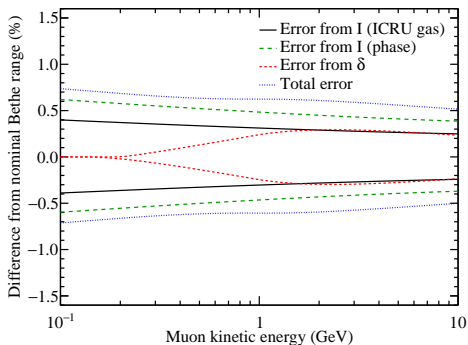
## Effect on muon range in DUNE



- Up to 0.5% error if we were to use exact treatment

## Total range uncertainty in DUNE

- $dE/dx$  is uncertain through the mean excitation energy  $I$  and the density effect
- Mean excitation energy error adopted by ICRU is  $188 \pm 10$  eV
- But only been measured in gas. Looking at few examples of substances measured in both liquid & gas, estimate 5% additional error for phase change



- Error on range is 0.6% across energies relevant to DUNE  $\nu_\mu$

## Is that big?

- In last NOvA analysis, took 0.9% error on muon range fully correlated ND/FD, and 0.27% uncorrelated
- Fully correl'd  $\Rightarrow \pm 0.010 \times 10^{-3} \text{ eV}^2$  in  $\Delta m_{32}^2$ ,  $\pm 0.0031$  in  $\sin^2 \theta_{23}$
- Uncorrelated  $\Rightarrow \pm 0.0015 \times 10^{-3} \text{ eV}^2$  in  $\Delta m_{32}^2$ ,  $\pm 0.0016$  in  $\sin^2 \theta_{23}$
- We're looking at 0.6% uncorrelated error from LAr alone (more later) plus a smaller (0.2%??) correlated error
- $\Rightarrow$  Very rough estimation (equating NOvA and DUNE)  $\pm 0.004 \times 10^{-3} \text{ eV}^2$  in  $\Delta m_{32}^2$ ,  $\pm 0.004$  in  $\sin^2 \theta_{23}$
- DUNE sensitivity claims (CDR, Nu2018 talk):
  - $\Delta m_{32}^2$ :  $\pm 0.004 \times 10^{-3} \text{ eV}^2$
  - $\sin^2 \theta_{23}$ : can be as good as  $\pm 0.002$  (depending on values of various oscillation parameters)
- **Potential to be a leading error** impacting  $\Delta m_{32}^2$  and **max-mixing discrimination**
- Obviously needs a study using DUNE sensitivities