in Fig. 7, yields

$$\tilde{A} = 2.40\times 10^{-46} \quad \text{and} \quad \tilde{B} = 1.55\times 10^{-46} \qquad (10)$$

or

$$\tilde{A} = -0.87\times 10^{-46} \quad \text{and} \quad \tilde{B} = 6.85\times 10^{-46} \,. \qquad (11)$$

The present analysis does not specify the correct pair of solutions. This ambiguity is similar to that encountered by Bloembergen and Rowland[3] in their analysis of thallium in the magnetic regime. As they point out, however, the relative strengths of the pseudo-exchange-coupling and the classical dipolar coupling increases from a ratio of 0.01 in the light elements such as the HD molecule to a ratio of 10 to 20 in the heavier metallic elements such as thallium. On this basis, the values $\tilde{A} = 2.40\times 10^{-46}$ and $\tilde{B} = 1.55\times 10^{-46}$ erg cm^3 are favored for indium. This results in $\tilde{A}/\tilde{B} = 6.8$.

The NQR for dilute alloys of tin in indium have also been measured. The problem of very broad alloy resonances precluded accurate reduction of the measured data since the Zeeman-modulated distribution exceeded the maximum scan width of the spectrometer (for a given marginal oscillator setting). However, the gross asymmetry of the alloy resonances was apparent from the as-recorded data, as seen in Fig. 8, and is in qualitative agreement with the results predicted by Thatcher[10] from his NMR data.

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

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This paper presents a simple reformulation of the expression for the density effect correction δ, i.e., the reduction in the ionization loss of fast charged particles due to the dielectric polarization of the medium. The general expression for δ 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.

I. INTRODUCTION

The density effect correction for the ionization loss of charged particles at high energies[1-7] has been previously evaluated for a large number of substances.[4-7] With the advent of the high-energy accelerators in the past decade, the need has arisen for the calculation of the density effect in a variety of additional materials (with various compositions and densities), which were not included in the previous work (Refs. 4-7). In these references, an appropriate dispersion oscillator model was constructed for each new material, and the resulting values of the density effect correction δ as a function of momentum p were then fitted with a four-parameter formula which was first introduced by Sternheimer in 1952. In this formula, δ is actually expressed as a function of X, defined by $X \equiv \log_{10}(p/m_0 c)$, where m_0 is the mass of the incident charged particle.

It was recently suggested by Berger[8] that in view of the growing demand for data on $\delta(X)$ for new materials, it would be of interest to obtain a general expression for $\delta(X)$, which would not require a detailed fitting procedure for each substance, if this is possible. After trying several possible fits, we have found such a general expression for the density effect correction $\delta(X)$. The expression 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 $< 2\%$, with the most likely errors being of the order of 1% or less, which is, in any case, of the order of the expected accuracy of the Bethe-Bloch formula.

In Sec. II, we derive the simplified expression for $\delta(X)$, and we give the prescription for obtaining the constants which enter into $\delta(X)$ for each of the four cases of interest, namely: (a) condensed materials (solids and liquids) with low atomic number Z ($Z \lesssim 8$) and (b) those with medium or high Z ($Z \gtrsim 8$); (c) gases having relatively low Z ($Z \lesssim 20$) and (d) gases having medium or high Z ($Z \gtrsim 20$).

In Sec. III, the general expression for $\delta(X)$ of Sec. II is used to simplify the expressions for the ionization loss [dE/dx, $(dE/dx)_{W_0}$, and ϵ_{prob}] in the region where the density effect correction is important.

Section IV gives the details of the calculation of δ for two illustrative examples. Finally, in Sec. V, we present a brief summary and discussion of the results obtained in the present paper.

II. GENERAL EXPRESSION FOR THE DENSITY EFFECT CORRECTION δ

The expression for $\delta(X)$ which was used in the previous work of Refs. 4–7 is as follows:

$$\delta = 4.606X + C + a(X_1 - X)^m \quad (X_0 < X < X_1)\,, \tag{1}$$

$$\delta = 4.606X + C \quad (X > X_1)\,, \tag{2}$$

where X_0 and X_1 are particular values of $X \equiv \log_{10} \times (p/m_0c)$, such that $\delta = 0$ for $X < X_0$, and for $X > X_1$, δ has reached its asymptotic form given by Eq. (2). Note that because of the definition of X, $4.606X$ is simply $2\ln(p/m_0c)$. In Eqs. (1) and (2), the constant C depends only on the mean excitation potential I and the density ρ_0 of the substance considered, where I is the average potential which enters into the Bethe-Bloch formula for dE/dx. Thus C can be calculated at once if the composition and the density of the substance (or the pressure and temperature in case of a gas) are known. The expression for C will be given below [see Eq. (3)]. In contrast to C, the constants a and m, which appear in Eq. (1), together with X_0 and X_1, are adjustable parameters whose values depend on the spectrum of dispersion frequencies ν_i and oscillator strengths f_i of the atoms of the material considered. In the present paper, we will give a simple prescription for obtaining a, m, X_0, and X_1 for any material (condensed substance or gas), provided only that the composition and density of the substance are known.

In connection with Eqs. (1) and (2), the constant C is given by

$$C = -2\ln(I/h\nu_p) - 1\,, \tag{3}$$

where I is the mean excitation potential for the electrons of the substance, and $h\nu_p$ is the corresponding plasma energy, with ν_p defined by

$$\nu_p = (ne^2/\pi m_e)^{1/2}\,, \tag{4}$$

where n is the electron density (number of electrons per cm^3), and m_e is the electron mass. From Eq. (4), one obtains[9]

$$h\nu_p = 28.8(\rho_0 Z/A_0)^{1/2}\ \text{eV} \tag{5}$$

for the value of $h\nu_p$ in electron volts; here ρ_0 is the density of the material (in g/cm^3), and Z and A_0 are the atomic number and atomic weight, respectively. In the case of a compound or mixture, the ratio Z/A_0 is to be replaced by the ratio of the total number of electrons to the effective molecular weight or sum of atomic weights: $\sum_i Z_i / \sum_i A_i$.

Referring to Eq. (1), the condition that $\delta(X_0) = 0$ actually determines the constant a, so that there are only three independent parameters, namely, X_0, X_1, and m. In order to obtain the equation for a in terms of X_0, X_1, and m, we write

$$\delta(X_0) = 0 = 4.606X_0 + C + a(X_1 - X_0)^m\,, \tag{6}$$

whence

$$a = (-C - 4.606X_0)/(X_1 - X_0)^m\,. \tag{7}$$

For simplicity of notation, since C is always negative [see Eq. (3)], we define $\bar{C} \equiv -C$. Furthermore, it is useful to introduce the value of X corresponding to C or $\bar{C}$, namely, X_a, defined as follows:

$$X_a \equiv \frac{-C}{4.606} = \frac{\bar{C}}{4.606} = \log_{10}\left(\frac{Ie^{1/2}}{h\nu_p}\right) = \log_{10}\left(\frac{1.649I}{h\nu_p}\right)\,. \tag{8}$$

Thus Eq. (7) becomes

$$a = 4.606(X_a - X_0)/(X_1 - X_0)^m\,. \tag{9}$$

Aside from this equation for a (which was implicitly used in the previous fits of Refs. 4–7), there is also a condition on m, which must be satisfied for any given values of X_0, X_1, and X_a. To obtain this condition, we differentiate Eq. (1), which gives

$$\frac{d\delta}{dX} = 4.606 - ma(X_1 - X)^{m-1}\,. \tag{10}$$

For physical reasons, this derivative must be positive, since the density effect correction δ always increases with increasing X (increasing momentum). Equation (10) shows that $d\delta/dX$ is smallest for $X = X_0$, since m and a are both positive (and $m > 1$), and hence $ma > 0$. From the requirement that $d\delta/dX > 0$ at $X = X_0$, we find that m must be less than a maximum value $m_{\max}$, which is determined by

$$m=\frac{4.606}{a(X_1-X_0)^{m-1}}=\frac{X_1-X_0}{X_a-X_0}\ . \tag{11}$$

In Eq. (11), X_a is, of course, determined by $\bar{C}$ [Eq. (8)], whereas X_0 and X_1 are still adjustable parameters. The value of $(X_1-X_0)/(X_a-X_0)$ will be denoted by $m_{\max}$ in the following discussion, and we must have $m \leqq m_{\max}$.

Before proceeding to a determination of the parameters m, X_0, and X_1, we note that upon inserting Eqs. (8) and (9) into Eq. (1), we obtain the alternative expression for δ

$$\delta=4.606(X-X_a)+4.606(X_a-X_0)[(X_1-X)/(X_1-X_0)]^m\ . \tag{12}$$

This form of Eq. (1), of course, shows at once that $\delta(X_0)=0$.

In order to proceed with the determination of m, X_0, and X_1 for the various physical cases (condensed materials and gases), we consider the detailed fits which have been previously obtained,[4-7] particularly those of Refs. 6 and 7. In these latter two references and also in the present work, we use the expression for the mean excitation potential I (divided by Z), which was proposed by Sternheimer,[6] on the basis of measurements for $Z \geqq 13$ (in particular, aluminum, copper, and lead). We have

$$I/Z=9.76+58.8Z^{-1.19}\ \text{eV}\ . \tag{13}$$

The sum of the first two terms of δ in Eq. (1), namely,

$$\delta_0 \equiv 4.606X+C=4.606(X-X_a)\ , \tag{14}$$

corresponds to the asymptotic expression for δ, also given by Eq. (2). The last term of Eq. (1), which will be approximated in the present work, will be denoted by δ_1. Thus,

$$\delta_1=a(X_1-X)^m\ . \tag{15}$$

The problem is that if we approximate the power function (monomial) δ_1 [Eq. (15)] by a different monomial of the same type, a certain error will be introduced as a function of X, and we want to make this error as small as possible. If the approximating function has parameters distinguished by being barred quantities, we have

$$\bar{\delta}_1=\bar{a}(\bar{X}_1-X)^{\bar{m}}, \tag{16}$$

where, of course, $\bar{a}$ is determined by an equation similar to (9), namely,

$$\bar{a}=4.606(X_a-\bar{X}_0)/(\bar{X}_1-\bar{X}_0)^{\bar{m}}, \tag{17}$$

where $\bar{a}$, $\bar{X}_0$, $\bar{X}_1$, and $\bar{m}$ are the parameters pertaining to the approximation $\bar{\delta}_1$ for δ_1. The error $\Delta(X)$ is given by

$$\Delta(X)=\bar{\delta}_1(X)-\delta_1(X)\ . \tag{18}$$

We note that in Eq. (17) the symbol X_a is not barred, since it is directly related to C [Eq. (8)], and this does not depend on the parameters of the approximation used for δ_1, and hence for $\delta=\delta_0+\delta_1$.

The calculations of $\Delta(X)$ were carried out on a computer. For each substance, we calculated $\delta_1(X)$ and the approximating functions $\bar{\delta}_1(X)$ for a variety of choices of $\bar{X}_0$, $\bar{X}_1$, and m. Of course, in each case, $\bar{a}$ was determined from Eq. (17). (C and hence X_a was included in the input.) For each case, δ_1 and the approximations $\bar{\delta}_1$ were calculated for a variety of X values ranging from X_0 to X_1 at intervals of 0.1 or 0.2 in X. The resulting differences $\Delta(X)$ [Eq. (18)] were also tabulated.

Even in the preliminary trial runs of the calculation, it was noticed that the value $\bar{m}=3.0$ gives a very good approximation to δ_1 throughout the range of Z values and both for condensed media and for gases. (The only exceptions are gaseous and liquid hydrogen and helium, for which the appropriate direct fits have been calculated and can be used. These exceptional cases will be discussed below.)

In order to obtain reliable values for the approximating parameters $\bar{X}_0$, $\bar{X}_1$, and $\bar{m}$, it was essential to have exact fits available for a wide range of substances, using the present values of I, as given by Eq. (13). This is in contrast to the fits obtained in Refs. 4 and 5, which pertained to I values which are, respectively, smaller and larger than the present values of I.

In connection with these exact fits, we note that the density effect correction δ is obtained from the following equations which were derived in Ref. 4:

$$\delta=\textstyle\sum_i f_i \ln[(l_i^2+l^2)/l_i^2]-l^2(1-\beta^2)\ , \tag{19}$$

where l is the solution of the equation

$$1/\beta^2-1=\textstyle\sum_i f_i/(l_i^2+l^2)\ . \tag{20}$$

In Eqs. (19) and (20), β is the velocity of the particle (in units c), f_i is the oscillator strength pertaining to the ith shell of the atom, and l_i is a dimensionless frequency pertaining to i. The determination of l_i has been discussed in detail in Ref. 6. Here we will merely give the expression for l_i. We have

$$l_i=h\nu_i'/h\nu_p=h\nu_i\rho/h\nu_p\ , \tag{21}$$

where $h\nu_i$ is the atomic ionization potential pertaining to the ith shell, $h\nu_i'$ is an effective excitation potential pertaining to i, which is given by $h\nu_i'=h\nu_i\rho$, where ρ is a multiplicative factor ($\rho>1$), which takes into account the possibility of excitation to continuum states. The value of ρ is determined by the condition that the geometric mean of the excitation energies $h\nu_i'$ be equal to I. Thus

$$\textstyle\sum_i f_i \ln(h\nu_i')=\sum_i f_i \ln(h\nu_i\rho)=\ln I\ . \tag{22}$$

TABLE I. Data used to calculate the density effect for the substances listed in Table II. The values of $h\nu_i$ are in Ry.

Material	N	Ne	Ar	Cu	Br	Kr	Ag	Xe	Pb	U
$h\nu_1$	29.4	64.0	235.3	661.4	993	1055	1879	2547	6469	8515
$h\nu_2$	3.0	3.0	19.4	72.1	120	129	258.5	370	1053	1418
$h\nu_3$	1.4		3.0	5.5	12	11.4	35.4	60.7	215	306
$h\nu_4$				1.0	2	3.0	4.0	7.6	28.2	51.7
$h\nu_5$								2.0	4.3	11.7
$h\nu_6$									2.0	2.0
f_1	$\frac{2}{7}$	$\frac{2}{10}$	$\frac{2}{18}$	$\frac{2}{29}$	$\frac{2}{35}$	$\frac{2}{36}$	$\frac{2}{47}$	$\frac{2}{54}$	$\frac{2}{82}$	$\frac{2}{92}$
f_2	$\frac{2}{7}$	$\frac{8}{10}$	$\frac{8}{18}$	$\frac{8}{29}$	$\frac{8}{35}$	$\frac{8}{36}$	$\frac{8}{47}$	$\frac{8}{54}$	$\frac{8}{82}$	$\frac{8}{92}$
f_3	$\frac{3}{7}$		$\frac{8}{18}$	$\frac{18}{29}$	$\frac{18}{35}$	$\frac{18}{36}$	$\frac{18}{47}$	$\frac{18}{54}$	$\frac{18}{82}$	$\frac{18}{92}$
f_4				$\frac{1}{29}$	$\frac{7}{35}$	$\frac{8}{36}$	$\frac{19}{47}$	$\frac{18}{54}$	$\frac{32}{82}$	$\frac{32}{92}$
f_5								$\frac{8}{54}$	$\frac{18}{82}$	$\frac{18}{92}$
f_6									$\frac{4}{82}$	$\frac{14}{92}$
$\langle h\nu_m\rangle$ (eV)	56.5	75.2	151.9	199.7	248.5	254.2	331.4	373.9	566.6	676.3
ρ	1.558	1.729	1.382	1.617	1.497	1.499	1.470	1.484	1.458	1.365
I (eV)	88	130	210	323	372	381	487	555	826	923

In Eq. (21), the denominator $h\nu_p$ is the plasma energy for the stopping medium, as given by Eq. (5).

In the present work, we have obtained very accurate fits to δ [Eq. (19)] for 12 substances (with the aid of a desk computer), using the Eqs. (1) and (2) with freely adjustable a, m, X_0, and X_1. The effective ionization potentials $h\nu_i$, which were used in the calculations, were obtained by means of standard tabulations.[10,11] The values of $h\nu_i$, f_i, and the resulting mean value $\langle h\nu_m\rangle$ are given in Table I. We note that $\langle h\nu_m\rangle$ is given by

$$\textstyle\sum_i f_i \ln(h\nu_i) = \ln\langle h\nu_m\rangle \ . \tag{23}$$

Thus, from Eqs. (22) and (23), we see that ρ is determined by the equation

$$\rho = I/\langle h\nu_m\rangle \ . \tag{24}$$

At the bottom of Table I, we have listed the values of ρ and I. We note that in the calculations of δ, besides the data of Table I of the present paper, values of $h\nu_i$, f_i, ρ, and I were also taken from Tables I of Refs. 6 and 7. For $Z \geqq 13$, we have used Eq. (13) for I. For the two cases with lower Z, namely, N and Ne, we have used values of I close to $I = 13Z$ eV. The actual choices of $I_{\rm N} = 88$ eV and $I_{\rm Ne} = 130$ eV were obtained from a consideration of the compilations of Berger and Seltzer[12] and of Turner *et al.*[13]

The substances for which accurate fits for δ were obtained are as follows: (a) condensed materials: a liquid H_2-Ne mixture used in a bubble-chamber experiment (with composition 83.05-at.% H, 16.95-at.% Ne)[14]; Cu, AgBr, Pb, and U; (b) gases (at 0 °C, normal pressure): H_2, He, N_2, Ne, Ar, Kr, and Xe. The resulting values of the parameters C, a, m, X_0, and X_1 are listed in Table II. For completeness, this table also includes the results for liquid hydrogen ($\rho_0 = 0.060$ g/cm^3) obtained in Ref. 7. The fit of Eq. (1) to the values of δ of Eq. (19) was within 0.10 at all momenta, the average absolute deviation at five or six selected momenta being ~0.05. (The same type of accuracy was also previously obtained in Refs. 6 and 7.) For comparison, the square bracket of the formula for dE/dx is of the order of 20 (see Sec. III), so that a deviation of 0.10 corresponds to ~0.5% accuracy in dE/dx.

Table II also gives the values of ρ_0, I, $h\nu_p$, and the parameters A and B for each substance, where A and B are defined by[4-7]

$$A \equiv 2\pi m e^4/m_e c^2 \rho_0 = 0.1536(Z/A_0) \text{ MeV/g cm}^{-2} \ , \tag{25}$$

$$B \equiv \ln[m_e c^2 (10^6 \text{ eV})/I^2] . \tag{26}$$

As noted above, the density ρ_0 for the gases corresponds to "normal temperature and pressure" (0 °C, 1 atm), for which the calculations were carried out. The effect on δ of changing the density ρ_0 for any material (especially for gases) will be discussed below. We note that for H_2, we used the I value ($I = 18.7$ eV) given by Berger and Seltzer.[12]

The cases of hydrogen and helium represent exceptions, because the dispersion model consists of a single type of dispersion oscillator (with frequency I/h). Since accurate fits are given in Table II, these cases will not be considered in connection with the search for an acceptable fit for δ for the other substances.

Considering Table II of this paper, and the Tables II of Refs. 6 and 7, we note that for the condensed materials, we have $X_1 = 2.0$ for the substances with $I < 100$ eV, and $X_1 = 3.0$ for the substances with $I > 100$ eV. [The only exception is the H_2-Ne liquid mixture with low density ($\rho_0 = 0.253$ g/cm^3) for which $X_1 = 3.0$, even though $I = 68.7$ eV is less than 100 eV. However, this is probably an unusual case, because of the low density and the large percentage of hydrogen atoms (83%).]

For the gases N_2, Ne, and Ar, we have $X_1 = 4.0$, whereas for the two "heavier" gases Kr and Xe, we find $X_1 = 5.0$. We also note in Table II of Ref. 5, that for the "light" gases CH_4, $(CH_2)_2$, $(CH)_2$, and CO_2, all of which have $\overline{C}$ values below that of N_2, we again have $X_1 = 4.0$.

In view of these results, we propose that in the general expression for $\delta(X)$, the following values of $\overline{X}_1$ be used:

(a) for condensed materials (solids and liquids):

$$\overline{X}_1 = 2.0 \quad \text{for } I < 100 \text{ eV} , \tag{27}$$

$$\overline{X}_1 = 3.0 \quad \text{for } I \geqq 100 \text{ eV} ; \tag{28}$$

(b) for gases under normal conditions (0 °C; 1 atm):

$$\overline{X}_1 = 4.0 \quad \text{for } \overline{C} < 12.25 , \tag{29}$$

$$\overline{X}_1 = 5.0 \quad \text{for } \overline{C} \geqq 12.25 . \tag{30}$$

The dividing value of $\overline{C} = 12.25$ was chosen because argon, for which $\overline{C} = 12.098$ (see Table II), is actually a limiting case, with $X_1 = 5.0$ giving almost as good a fit as $X_1 = 4.0$.

Concerning the value of $\overline{m}$, as has been mentioned above, the use of $\overline{m} = 3.0$ gives a very good fit to the actual $\delta(X)$, for all cases (condensed materials and gases), except for hydrogen and helium. The possibility of a good fit using $\overline{m} = 3.0$ is suggested by the actual values of m for the detailed fits in Tables II of Refs. 6 and 7, and the present paper. Thus the values of m range from 2.539 for CsI to 4.615 for Al_2O_3, with most of the m values lying between ~2.5 and 3.5.

The actual maximum deviations $\Delta_{\max}$ [see Eq. (18)] were obtained by computing $\Delta(X)$ with $\overline{m} = 3.0$ for a total of 22 condensed materials (17 solids and 5 liquids) and for 9 gases at normal conditions. Besides $\overline{m} = 3.0$, and the $\overline{X}_1$ values given by Eqs. (27)–(30), we used values of $\overline{X}_0$ which will be discussed below. The corresponding values of $\overline{a}$ were calculated from Eq. (17).

The average absolute maximum deviation $\langle |\Delta_{\max}| \rangle$, i.e., the average of the $|\Delta_{\max}|$ values, is 0.178 for the solids and liquids and 0.175 for the gases. The largest of the $\Delta_{\max}$ values occurs for the H_2-Ne mixture with density $\rho_0 = 0.8$ g/cm^3, and it is only 0.381. When this is compared to the value of the square bracket in the Bethe-Bloch

TABLE II. Values of the constants which enter into the expression for the ionization loss [Eq. (55)] and the density effect correction δ [Eqs. (1) and (2)]. The mean excitation potential I and the plasma energy $h\nu_p$ are in eV, and A is in units MeV/g cm^{-2}. The values of C, a, m, X_0, and X_1 enter into Eqs. (1) and (2).

Material	ρ_0	I	$h\nu_p$	A	B	$-C$	a	m	X_0	X_1
H_2-Ne	0.253	68.70	11.16	0.09110	18.500	4.636	0.06240	3.971	0.442	3.0
Cu	8.96	323.0	58.23	0.07010	15.404	4.427	0.1004	3.450	0.207	3.0
AgBr	6.473	434.0	48.42	0.06708	14.814	5.387	0.06708	2.929	0.333	3.0
Pb	11.35	826.0	61.04	0.06079	13.527	6.211	0.3951	2.520	0.317	3.0
U	19.05	923.0	78.15	0.05937	13.304	5.939	0.3763	2.515	0.077	3.0
Liq. H_2	0.060	18.7	7.03	0.1524	21.103	2.96	0.0669	5.949	0.425	2.0
Gas H_2	0.08988×10^{-3}	18.7	0.2720	0.1524	21.103	9.463	0.4887	4.754	1.837	3.0
He	0.177×10^{-3}	42.0	0.2708	0.07675	19.484	11.090	2.008	3.297	2.191	3.0
N_2	1.2506×10^{-3}	88.0	0.720	0.07676	18.005	10.614	0.1730	3.311	1.769	4.0
Ne	0.8999×10^{-3}	130.0	0.6083	0.07611	17.225	11.731	0.3061	2.956	2.112	4.0
Ar	1.7837×10^{-3}	209.6	0.8165	0.06921	16.269	12.098	0.4338	2.730	2.010	4.0
Kr	3.733×10^{-3}	381.0	1.153	0.06599	15.074	12.603	0.05895	3.686	2.020	5.0
Xe	5.887×10^{-3}	555.0	1.417	0.06317	14.322	12.943	0.1158	3.175	1.837	5.0

formula for dE/dx [see Eq. (52)], which is usually larger than 20, the corresponding error in dE/dx is seen to be less than 2%, whereas the average error corresponding to $\langle|\Delta_{\max}|\rangle \sim 0.177$ is less than 1%. These errors are probably within the limits of error of the Bethe-Bloch formula, due to the uncertainty in the value of the mean excitation potential I.

In connection with the average maximum deviation $\langle|\Delta_{\max}|\rangle = 0.177$, we note that if we lump the data from all of the substances $(22+9=31)$ together, we find that in only three cases is $|\Delta_{\max}|$ between 0.3 and 0.4. In all other cases (28 altogether), $|\Delta_{\max}|$ lies below 0.3.

Upon setting $m=3$ in Eq. (11), we obtain an equation which can be solved for X_0. The resulting X_0, to be denoted by $X_{0,\min}$, is the smallest value of X_0 such that $m_{\max} \geqq 3$, i.e., for still smaller values of X_0 $(X_0 < X_{0,\min})$, $m_{\max}$ would be < 3, and a fit with $\bar{m}=3$ would not be possible.

We thus find

$$(X_1 - X_{0,\min})/(X_a - X_{0,\min}) = 3 \,, \tag{31}$$

whence,

$$X_{0,\min} = \tfrac{3}{2}X_a - \tfrac{1}{2}X_1 = 0.326\bar{C} - 0.5X_1 \,, \tag{32}$$

where we have used Eq. (8) for X_a.

We will now discuss the values of $\bar{X}_0$, which we shall propose in connection with the general expression for $\delta(X)$.

We consider first the condensed materials. We note from Tables II of Refs. 6 and 7 and of the present paper, that the values of X_0 for these substances are all in the general vicinity of $X_0 = 0.2$, with an effective spread from $X_0 \sim 0$ to $X_0 \sim 0.4$. We will therefore assume $\bar{X}_0 = 0.2$ for all solids and liquids, unless the value of $X_{0,\min}$ as determined from Eq. (32) exceeds 0.2, in which case $\bar{X}_0 = X_{0,\min}$ will be used. It should be pointed out that this prescription for $\bar{X}_0$ was used in obtaining the fits $\bar{\delta}_1(X)$, using $\bar{m}=3.0$, which were discussed above.

Since $X_{0,\min}$ is a function of X_1 and $\bar{C}$, the prescription that $X_{0,\min} \leqq 0.2$ takes the following form: *values of parameters for solids and liquids*:

(1) for $I < 100$ eV: $\bar{X}_1 = 2.0$, $\bar{m} = 3.0$;

$$\text{(a) } \bar{X}_0 = 0.2 \quad \text{for } \bar{C} < 3.681 \,, \tag{33}$$

$$\text{(b) } \bar{X}_0 = 0.326\bar{C} - 1.0 \quad \text{for } \bar{C} \geqq 3.681 \,; \tag{34}$$

(2) for $I \geqq 100$ eV: $\bar{X}_1 = 3.0$, $m = 3.0$;

$$\text{(a) } \bar{X}_0 = 0.2 \quad \text{for } \bar{C} < 5.215 \,, \tag{35}$$

$$\text{(b) } \bar{X}_0 = 0.326\bar{C} - 1.5 \quad \text{for } \bar{C} \geqq 5.215 \,. \tag{36}$$

We note that, with only one exception, for the cases with $I < 100$ eV, $\bar{C}$ was always less than 3.68, so that Eq. (34) applies only in exceptional cases, i.e., in general, $\bar{X}_0 = 0.2$ for substances with $I < 100$ eV. On the other hand, for $I \geqq 100$ eV, since $\bar{C}$ increases with increasing I, there exist cases for which Eq. (36) must be used rather than Eq. (35) $(X_0 = 0.2)$. In particular, in Table II of the present paper, we have $\bar{C} > 5.215$ for AgBr $(\bar{C} = 5.387)$, Pb $(\bar{C} = 6.211)$, and U $(\bar{C} = 5.939)$. The corresponding values of $\bar{X}_0$ [Eq. (36)] are $\bar{X}_0 = 0.256$, 0.525, and 0.436, respectively. Similarly, from Table II of Ref. 7, we note that $\bar{C} = 5.95$ for NaI and $\bar{C} = 6.29$ for CsI, which gives $\bar{X}_0 = 0.440$ and 0.551, respectively. We may note that the preceding values of $\bar{X}_0$ for AgBr, Pb, U, and CsI were used in obtaining the functions $\bar{\delta}_1(X)$ and the resulting $\Delta(X)$ [Eq. (18)].

Before proceeding to a discussion of the parameters $\bar{X}_0$ and $\bar{X}_1$ recommended for gases, we wish to comment on a minor point. In Refs. 5 and 6, one of us (R.M.S.) has used small but finite values of $\delta(X_0)$ for the case of metals, to take into account the small density effect provided by the conduction electrons at low energies. However, the values of $\delta(X_0)$ were always $\leqq 0.06$ (see Ref. 5, p. 514 and Ref. 6, p. 249). These values are so small that they can be safely neglected in the present work, and we have therefore chosen $\delta(X_0) = 0$ for all substances [see Eq. (6)].

The values of $\bar{X}_1$ and $\bar{m}$ for gases have already been determined [Eqs. (29) and (30)]. In order to obtain the values of $\bar{X}_0$ appropriate for the various regions of $\bar{C}$, we note from Table II of the present paper that for the gases above N_2 (i.e., Ne, Ar, Kr, and Xe), X_0 is generally close to 2.0, so that the choice $\bar{X}_0 = 2.0$ appears to be reasonable. For N_2, we have $X_0 = 1.769$, and for the "lighter" gases, namely, CH_4, $(CH_2)_2$, $(CH)_2$, and CO_2, Table II of Ref. 5 (see p. 514) indicates that X_0 is appreciably smaller than 2.0; in fact X_0 is of the order of 1.5 to 1.7. We note that the calculations of Ref. 5 for gases with low Z were carried out with essentially the same I values as those used in the present work. Thus in Ref. 5, we used $I_H = 19.0$ eV for H, and $I = 13Z$ eV for light elements $(Z \lesssim 10)$. From the values of $-C = \bar{C}$ in Table II of Ref. 5 (and also for N_2 and Ne in Table II of the present work), we arrive at the following prescription for $\bar{X}_0$ for gases with $Z \lesssim 10$:

$$\bar{X}_0 = 1.6 \quad \text{for } \bar{C} < 10.0 \,, \tag{37}$$

$$\bar{X}_0 = 1.7 \quad \text{for } 10.0 \leqq \bar{C} < 10.5 \,, \tag{38}$$

$$\bar{X}_0 = 1.8 \quad \text{for } 10.5 \leqq \bar{C} < 11.0 \,, \tag{39}$$

$$\bar{X}_0 = 1.9 \quad \text{for } 11.0 \leqq \bar{C} < 11.5 \,, \tag{40}$$

$$\bar{X}_0 = 2.0 \quad \text{for } 11.5 \leqq \bar{C} < 12.25 \,. \tag{41}$$

For the above regions of $\bar{C}$, we propose to use $\bar{m} = 3.0$, $\bar{X}_1 = 4.0$, as given above [Eq. (29)]. On the other hand, for $\overline{C} \geqq 12.25$, with $\overline{X}_1 = 5.0$, $\overline{m} = 3.0$, the value $\overline{X}_0 = 2.0$ will generally be adequate (see results for Ne, Ar, Kr, and Xe in Table II) unless $X_{0,\mathrm{min}} > 2.0$, as given by Eq. (32). This will occur only for $\overline{C} > 13.804$, which is essentially an academic case, since for Xe, $\overline{C} = 12.943$, and even for radon gas (Rn) with a density[11] $\rho_0 = 9.73 \times 10^{-3}$ g/cm^3, $\overline{C}$ is only 13.387, i.e., appreciably smaller than the limit of 13.804. It should be emphasized again that the above-mentioned values of $\overline{X}_0$, $\overline{X}_1$, and $\overline{C}$ all pertain to the gas at normal temperature (0 °C) and pressure (1 atm). The extension to other gas conditions is very simple and will be made below.

Summarizing the preceding discussion, we have obtained the following results for values of parameters for gases at normal conditions ($T = 0$ °C, $P = 1$ atm):

(a) $\overline{X}_1 = 4.0$, $\overline{m} = 3.0$ for $\overline{C} < 12.25$;

for values of $\overline{X}_0$ for the various regions of $\overline{C}$, see Eqs. (37)–(41),

(b) $\overline{X}_1 = 5.0$, $\overline{m} = 3.0$, $\overline{X}_0 = 2.0$ for $12.25 \leqq \overline{C} < 13.804$,

(c) $\overline{X}_1 = 5.0$, $\overline{m} = 3.0$, $\overline{X}_0 = 0.326\overline{C} - 2.5$ for $\overline{C} \geqq 13.804$. (42)

In order to obtain the corresponding values of the constants $\overline{C}$, $\overline{X}_0$, $\overline{X}_1$, and $\overline{m}$ when the gas is not at normal temperature and pressure (NTP), we make use of Eq. (11) of Ref. 4, namely,

$$\delta_P(P^{-1/2}p') = \delta_1(p') , \tag{43}$$

where $\delta_{P'}(\lambda)$ denotes the density effect correction δ for a pressure P' and momentum λ. In this equation, it was assumed that the temperature of the gas is the same at pressure P' as at pressure 1 atm. In general, if the *density* of the gas is η times that at NTP and we put $p = \eta^{-1/2}p'$, we obtain

$$\delta_\eta(p) = \delta_1(p\eta^{1/2}) , \tag{44}$$

where now δ_η is the value of δ at a density $\eta\rho_0$, where ρ_0 is the density at NTP [see also Eq. (18) of Ref. 6].

Thus we must evaluate δ_1 at a momentum $p\eta^{1/2}$ or at a value of $X_\eta \equiv X + \frac{1}{2}\log_{10}\eta$. We have

$$\delta_1(X + \tfrac{1}{2}\log_{10}\eta) = 4.606X + 2.303\log_{10}\eta + C + a(X_1 - X - \tfrac{1}{2}\log_{10}\eta)^m . \tag{45}$$

In the following, we will denote the parameters C, X_1, and X_0 by the additional subscript η, i.e., C_η, $X_{1,\eta}$, and $X_{0,\eta}$. (In this same notation, the previous parameters pertaining to $\eta = 1$ could be written as C_1, $X_{1,1}$, and $X_{0,1}$.)

Thus we shall define

$$C_\eta \equiv C + 2.303\log_{10}\eta , \tag{46}$$

$$X_{1,\eta} \equiv X_1 - \tfrac{1}{2}\log_{10}\eta , \tag{47}$$

$$X_{0,\eta} \equiv X_0 - \tfrac{1}{2}\log_{10}\eta . \tag{48}$$

Upon using Eqs. (46) and (47), Eq. (45) becomes

$$\delta_\eta(p) = \delta_1(X + \tfrac{1}{2}\log_{10}\eta) = 4.606X + C_\eta + a(X_{1,\eta} - X)^m , \tag{49}$$

and it is obvious that this expression applies for X between $X_{0,\eta}$ and $X_{1,\eta}$, i.e., $X_{0,\eta} \leqq X \leqq X_{1,\eta}$.

Since C is negative, and we have defined $\overline{C} \equiv -C$, we may also define $\overline{C}_\eta \equiv -C_\eta$. Equation (46) thus gives

$$\overline{C}_\eta = \overline{C} - 2.303\log_{10}\eta . \tag{50}$$

It is obvious from Eqs. (45) and (49), that the values of m and a are unchanged in going to a different density $\eta\rho_0$; thus, $m = 3.0$ independent of η. It may also be noted that Eqs. (46)–(49) obviously also apply to a condensed substance (solid or liquid) whose density has been changed (e.g., by compression) from the normal density ρ_0, which was assumed in obtaining the values of Eqs. (33)–(36).

Finally, we note that in all cases [Eqs. (33)–(49)], since $m = 3.0$, the value of a is obtained from [cf. Eq. (9)]

$$a = 4.606(X_a - X_0)/(X_1 - X_0)^3 , \tag{51}$$

where X_a is given by Eq. (8) (and for $\eta \neq 1$, $X_a = \overline{C}_\eta/4.606$).

In Sec. IV, we will give two illustrative examples of the calculation of δ, using Eqs. (33)–(51).

III. EXPRESSIONS FOR THE IONIZATION LOSS dE/dx

In this section, we will give simplified expressions for the energy loss dE/dx for various physical cases, in the region where the density effect is appreciable, i.e., for $X > X_0$. In obtaining these expressions, we will make use of the general expression for δ obtained in Sec. II.

We shall consider three cases of physical interest: (a) the average energy loss dE/dx, including all energy transfers W, i.e., up to $W = W_{\mathrm{max}}$; (b) the restricted ionization loss $(dE/dx)_{W_0}$, i.e., restricted to energy transfers less than some preassigned value W_0; (c) the most probably energy loss ϵ_{prob} in a thin absorber, as obtained from a slight modification of the Landau formula.[15]

(a) The average energy loss $-(1/\rho_0)(dE/dx)$ is given by the Bethe-Bloch formula,[16,17] modified for the existence of the density effect

$$-\left(\frac{1}{\rho_0}\right)\left(\frac{dE}{dx}\right) = \frac{2\pi n e^4}{m_e v^2 \rho_0}\left[\ln\left(\frac{2m_e v^2 W_{\mathrm{max}}}{I^2(1-\beta^2)}\right) - 2\beta^2 - \delta\right] , \tag{52}$$

where the maximum energy transfer $W_{\max}$ from the incident particle (mass m_0) to an atomic electron (mass m_e) is given by[18]

$$W_{\max}=\frac{p^2}{m_0(m_0/2m_e+m_e/2m_0+E/m_0c^2)}\quad, \tag{53}$$

where E and p are the total energy and momentum of the incident particle. We note that Eq. (53) reduces to

$$W_{\max}\simeq 2m_e v^2/(1-\beta^2)\quad\text{for } E\ll(m_0^2/2m_e)c^2\ . \tag{54}$$

As was shown in Ref. 4, in terms of the constants A and B [Eqs. (25) and (26)], Eq. (52) can be rewritten as

$$-\frac{1}{\rho_0}\frac{dE}{dx}=\frac{A}{\beta^2}\left[B+0.693+2\ln\left(\frac{p}{m_0c}\right)+\ln W_{\max}-2\beta^2-\delta\right]\ , \tag{55}$$

where $W_{\max}$ is in MeV, and the formula gives the energy loss in units MeV/g cm^{-2}.

We now consider the region $X_0\leqq X\leqq X_1$, where the density effect δ has not yet reached saturation. Since $2\ln(p/m_0c)=4.606X$, the square bracket of Eq. (55), to be denoted by F, can be written as follows in view of Eq. (1):

$$F=F_1-F_2\quad, \tag{56}$$

where

$$F_1=B+\overline{C}+0.693-2\beta^2+\ln W_{\max}\ , \tag{57}$$

$$F_2=a(X_1-X)^3\ , \tag{58}$$

where $W_{\max}$ is in MeV, and a is given by Eq. (51). Note that in Eq. (57), for $\beta\to 1$, we obtain $0.693-2\beta^2=-1.307$.

Of course, for $X\geqq X_1$, we have simply $F=F_1$, corresponding to Eq. (2).

(b) The restricted ionization loss $(-1/\rho_0)\times(dE/dx)_{W_0}$ for maximum energy transfer W_0 is given by[19]

$$-\left(\frac{1}{\rho_0}\right)\left(\frac{dE}{dx}\right)_{W_0}=\frac{2\pi ne^4}{m_e v^2\rho_0}\left[\ln\left(\frac{2mv^2W_0}{I^2(1-\beta^2)}\right)-\beta^2-\delta\right]\ . \tag{59}$$

In terms of the constants A and B, we obtain

$$-\left(\frac{1}{\rho_0}\right)\left(\frac{dE}{dx}\right)_{W_0}=\frac{A}{\beta^2}\left[B+0.693+2\ln\left(\frac{p}{m_0c}\right)+\ln W_0-\beta^2-\delta\right], \tag{60}$$

where W_0 is in units of MeV.

In the region $X_0\leqq X\leqq X_1$, the square bracket, to be denoted by F_{W_0}, can be written as $F_{1,W_0}-F_2$, where F_{1,W_0} is given by

$$F_{1,W_0}=B+\overline{C}+0.693-\beta^2+\ln W_0 \tag{61}$$

(W_0 in MeV). Of course, F_2 is again given by Eq. (58) for $X<X_1$, and it is zero for $X\geqq X_1$.

(c) The equation for the most probably loss ϵ_{prob} in a thin absorber was first derived by Landau[15] in 1944. It was recently shown by Maccabee and Papworth[20] that a term 0.373 in the original Landau formula is in error and should be replaced by 0.198. If t is the thickness of the absorber (in g/cm^2), we obtain

$$\epsilon_{\text{prob}}=\frac{2\pi ne^4t}{m_e v^2\rho_0}\left[\ln\left(\frac{2m_e v^2(2\pi ne^4t/m_e v^2\rho_0)}{I^2(1-\beta^2)}\right)-\beta^2+0.198-\delta\right]\ . \tag{62}$$

In terms of A and B, Eq. (62) can be written as

$$\epsilon_{\text{prob}}=(At/\beta^2)[B+0.891+2\ln(p/m_0c)+\ln(At/\beta^2)-\beta^2-\delta]\ , \tag{63}$$

where $0.891=\ln 2+0.198$.

In the region $X_0\leqq X\leqq X_1$, the square bracket of Eq. (63) to be denoted by F_{prob} can be written as $F_{1,\text{prob}}-F_2$, where $F_{1,\text{prob}}$ is given by

$$F_{1,\text{prob}}=B+\overline{C}+0.891-\beta^2+\ln(At/\beta^2)\ . \tag{64}$$

F_2 is again given by Eq. (58). For $X>X_1$, we have $F_2=0$, and $0.891-\beta^2\cong-0.109$.

In connection with our earlier statement that the values of the square bracket F of the formula for dE/dx are of the order of 20 or more [see discussion of $\Delta_{\max}$ values following Eq. (30)], we may note the following values of F for three materials: Be, Al, and Pb. These values were obtained by means of the tables of Sternheimer[21,22] for dE/dx of protons in the relativistic region. Thus[21] for Be, $F=22.06$ at $T_p=3.0$ BeV (T_p is the proton kinetic energy), which corresponds to the minimum of dE/dx; furthermore, $F=24.77$ at $T_p=10$ BeV, and $F=26.26$ at $T_p=20$ BeV. For Al, the corresponding values[21] are $F=20.15$ at $T_p=2.5$ BeV, $F=23.59$ at 10 BeV, and $F=25.30$ at 20 BeV. Finally[22] for the case of Pb, the corresponding results are $F=16.72$, 21.34, and 23.31 at $T_p=2.0$ (ionization minimum), 10, and 20 BeV, respectively. Although the values of F involved for $(dE/dx)_{W_0}$ and ϵ_{prob} will be slightly smaller than the above values which pertain to the average energy loss dE/dx, nevertheless the average estimate that F will be of the order of 20 is justified. This result leads to an average error of ~1% in dE/dx, due to the use of $m=3.0$, as discussed above in Sec. II.

IV. TWO ILLUSTRATIVE EXAMPLES

In order to illustrate the use of the equations for δ and dE/dx in Secs. II and III, we shall present the details of the calculations for two examples, namely, (a) the calculation of δ for methane (CH_4) at a pressure $P = 20$ atm, $T = 20\ ^\circ C$; (b) the calculation of the most probable loss ϵ_{prob} in a sample of tungsten (W) of thickness $t = 10$ g/cm^2, as a function of the energy E of the incident particle.

(a) In order to obtain δ for methane, using the equations of Sec. II, we calculate the mean excitation potential I for CH_4, based on $I_C = 13Z = 78$ eV for carbon,[5] and $I_H = 18.7$ eV for hydrogen.[12] Since there are six electrons per carbon atom and four electrons for the hydrogen in CH_4, we have

$$\log I_{CH_4} = \tfrac{6}{10}\log 78 + \tfrac{4}{10}\log 18.7\ , \tag{65}$$

whence $I_{CH_4} = 44.06$ eV. The density of CH_4 at NTP is $\rho_0 = 0.7168 \times 10^{-3}$ g/cm^3. With $\sum Z_i = 10$, $\sum A_i = 16.04$ (molecular weight), Eq. (5) gives (at NTP)

$$h\nu_p = 28.8(0.7168\times 10^{-3}\times 10/16.04)^{1/2} = 0.6088 \text{ eV}\ . \tag{66}$$

Upon inserting the values of I and $h\nu_p$ into Eq. (3), we obtain $-C = 9.565$. Similarly, Eqs. (25) and (26) give $A = 0.09575$ MeV/g cm^{-2} and $B = 19.389$.

We first obtain the density effect δ at NTP. Note that $\bar{C} = 9.565$ also pertains to NTP. For this value of $\bar{C}$, Eq. (37) gives $X_0 = 1.6$. From the list of parameters in Sec. II, we further obtain $X_1 = 4.0$ and $m = 3.0$. (Note that we have omitted the bar above each of these symbols, for simplicity, except for $\bar{C}$.)

From $\bar{C} = 9.565$, we obtain $X_a = 9.565/4.606 = 2.077$. Thus Eq. (51) gives

$$a = 4.606(2.077 - 1.6)/(4 - 1.6)^3 = 0.1589\ . \tag{67}$$

As noted in Sec. II, the values of a and m are independent of the density ρ_0.

For NTP, δ would be given by

$$\delta = 4.606X - 9.565 + 0.1589(4 - X)^3 \quad (1.6 \leqq X \leqq 4.0)\ . \tag{68}$$

For $P = 20$ atm and $T = 20\ ^\circ C$, η (the factor by which the density ρ_0 is multiplied) is given by

$$\eta = 20(273/293) = 18.63\ , \tag{69}$$

whence $\frac{1}{2}\log_{10}\eta = 0.635$, and $2.303\log_{10}\eta = 2.925$. Thus from Eq. (46)

$$C_\eta = -9.565 + 2.925 = -6.640\ , \tag{70}$$

and from Eqs. (47) and (48)

$$X_{1,\eta} = 4 - 0.635 = 3.365\ , \tag{71}$$

$$X_{0,\eta} = 1.6 - 0.635 = 0.965\ . \tag{72}$$

Finally, from Eq. (49), $\delta_\eta(\eta = 18.63)$ is given by

$$\delta_\eta = 4.606X - 6.640 + 0.1589\ (3.365 - X)^3 \quad (0.965 \leqq X \leqq 3.365)\ . \tag{73}$$

Of course, $\delta_\eta = 0$ for $X < 0.965$, and for $X > 3.365$, the last term in Eq. (73) is to be omitted.

Thus Eq. (73) is the desired equation for δ of methane at 20 atm.

In connection with the behavior of δ as a function of $X = \log_{10}(p/m_0c)$, we have shown in Fig. 1 the values for δ for neon (at NTP), using $m = 3.0$. With $\bar{C} = 11.731$ for Ne (see Table II), this gives $X_a = 2.547$ and $X_0 = 2.0$ from Eq. (41), and $X_1 = 4.0$ (see Sec. II). The resulting value of a [Eq. (51)] is $a = 0.3149$. Thus δ is given by

$$\delta = 4.606X - 11.731 + 0.3149\ (4 - X)^3 \quad (2.0 \leqq X \leqq 4.0). \tag{74}$$

The curve of $\delta(X)$ vs X is shown in Fig. 1, together with the "asymptotic" values δ_{asympt}, obtained by omitting the last term in Eq. (74). The values of X_0, X_a, and X_1 are also marked on this figure. Obviously, the difference between δ and δ_{asympt} (broken line) is given by the cubic term of Eq. (74). δ_{asympt} would obviously be negative at $X = X_0 = 2.0$, and the equation for a [Eq. (51)] is determined by the condition that the total δ shall be zero at $X = X_0$.

(b) The second example considered in this section concerns the density effect in metallic tungsten, and the most probable energy loss ϵ_{prob} in a

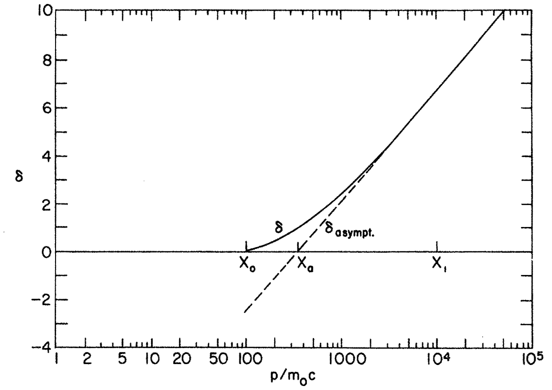

FIG. 1. The density effect correction δ for neon gas (at normal temperature and pressure) as a function of p/m_0c of the incident particle. The solid curve gives δ [Eq. (1)], while the broken straight line represents the asymptotic relation δ_{asympt} of Eq. (2), which has been extended down to $X = X_0$. The cubic term of Eq. (1) (with $m = 3.0$) represents the difference between δ and δ_{asympt} [denoted by δ_1 in Eq. (15)]. We have $X_0 = 2.0$, $X_a = 2.547$, and $X_1 = 4.0$, corresponding to $p/m_0c = 100$, 352, and 10^4, respectively.

sample of thickness $t=10$ g/cm^2.

In order to obtain the mean excitation potential I, we use Eq. (13) with $Z=74$. This gives $I=748$ eV. With a density[11] $\rho_0=19.35$ g/cm^3 and atomic weight $A_0=183.85$, Eq. (5) yields $h\nu_p=80.38$ eV, and hence [from Eq. (3)], $\overline{C}=-C=5.462$, so that $X_a=1.186$.

From Eq. (36), we find $X_1=3.0$, $m=3.0$, and (since $\overline{C}>5.215$)

$$X_0=(0.326)(5.462)-1.5=0.281\ . \tag{75}$$

The resulting value of a is

$$a=\frac{4.606(X_a-X_0)}{(X_1-X_0)^3}=\frac{(4.606)(1.186-0.281)}{(3-0.281)^3}=0.2074\ . \tag{76}$$

Thus we obtain for δ

$$\delta=4.606X-5.462+0.2074\,(3-X)^3 \qquad (0.281\leqq X\leqq 3)\ . \tag{77}$$

From Eqs. (25) and (26), we obtain $A=0.06182$ MeV/g cm^{-2} and $B=13.725$. Note that $X_0=0.281$ corresponds to $p/m_0c=10^{0.281}=1.910$, and $E/m_0c^2=2.156$ (E is the total energy including rest mass). Similarly, $X_a=1.186$ gives $p/m_0c=10^{1.186}=15.35$, and $E/m_0c^2=15.38$.

With $t=10$ g/cm^2, we find $At=0.6182$ MeV, $\ln At=-0.4810$. Thus we obtain

$$\epsilon_{\text{prob}}=\frac{0.6182\text{ MeV}}{\beta^2}\left[B+0.891+2\ln\left(\frac{p}{m_0c}\right)-0.481-\ln\beta^2-\beta^2-\delta\right]\ . \tag{78}$$

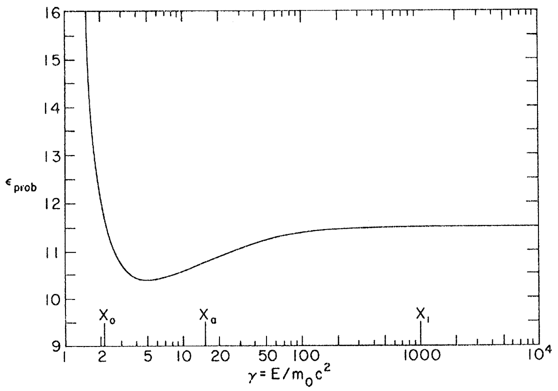

FIG. 2. The most probable energy loss ϵ_{prob} [Eq. (62)] in a sample of tungsten of thickness $t=10$ g/cm^2, as a function of $\gamma=E/m_0c^2$ of the incident particle. The values of X_0, X_a, and X_1 correspond to values of $\gamma=2.156$, 15.38, and 10^3, respectively. The minimum of ϵ_{prob} occurs at $\gamma=5.0$, and the relativistic rise is from 10.38 MeV (at minimum) to 11.50 MeV (plateau value, attained for $\gamma\gtrsim 10^3$).

In the region $0.281\leqq X\leqq 3.0$, the square bracket F_{prob} of Eq. (78) can be written as $F_{1,\text{prob}}-F_2$, where F_2 is the cubic term of Eq. (77), and $F_{1,\text{prob}}$ is given by

$$\begin{aligned}F_{1,\text{prob}}&=B+\overline{C}-0.109+(1-\beta^2)-0.481-\ln\beta^2\\&=18.597+(1-\beta^2)-\ln\beta^2\ .\end{aligned} \tag{79}$$

Thus at very high energies, i.e., $X>X_1=3.0$, we find

$$\epsilon_{\text{prob}}(X>3.0)=0.6182\times 18.597=11.497\text{ MeV}. \tag{80}$$

Note that when β^2 is very close to 1, so that $\beta^2=1-\epsilon$, where $\epsilon\ll 1$, the term $(1-\beta^2)-\ln\beta^2$ in Eq. (79) approaches simply 2ϵ.

For $0.281\leqq X\leqq 3.0$, ϵ_{prob} was obtained from Eqs. (78) and (79). We note that the minimum of ϵ_{prob} occurs at $\beta=0.980$ ($\gamma\cong 5.0$), the resulting value being $\epsilon_{\text{prob}}(\text{min})=10.381$ MeV. Thus the relativistic rise is only a factor of $11.497/10.381=1.108$. The smallness of the relativistic rise of ϵ_{prob} for condensed materials has been previously discussed in Refs. 4 and 5. It is obviously due to the great importance of the density effect, which results from the large electronic density n.

For $X<0.281$, we have $\delta=0$, and ϵ_{prob} was calculated directly from Eq. (78). Altogether, 20 calculations of ϵ_{prob} were carried out throughout the range of momenta. The resulting curve of ϵ_{prob} as a function of $\gamma=E/m_0c^2$ is shown in Fig. 2. The values of γ corresponding to X_0, X_a, and X_1 are also shown in this figure.

V. SUMMARY AND DISCUSSION

We have obtained a simple reformulation of the density effect correction δ, starting from Eqs. (1) and (2), and from the previous fits for δ obtained in Refs. 4–7 for a large number of substances. Thus it was found that in the term $a(X_1-X)^m$ of δ [Eq. (1)], it is adequate to use $m=3.0$ for all substances. With a proper choice of X_0 and X_1, this value of m gives an accuracy of better than 2% in dE/dx throughout the range of momenta. We note that the factor a in the above expression is not a free parameter, but is determined uniquely by X_0, X_1, and X_a (which is directly related to C) [see Eqs. (8) and (51)]. The values of X_0 and X_1 depend upon the type of substance considered, i.e., essentially on the density ρ_0 and the atomic number Z. Prescriptions for obtaining X_0 and X_1 for the various regions of ρ_0 and Z have been given in Eqs. (27)–(30) and (33)–(42). Thus it is possible to obtain δ by a simple procedure for any material (e.g., nuclear emulsion or biological materials, such as muscle and bone) if the density and the composition are known. The latter determines the mean excitation potential I. In the present work, we have used the I values given by Eq. (13), which was proposed by one of us (R.M.S.) in Ref. 6 This equation fits the experimentally determined I values in the region of $Z \geqq 13$. For smaller Z, the I values suggested by Berger and Seltzer[12] can be used. We note that as an alternative to the preceding I values, the values of Turner *et al.*[13] can also be employed. The latter values tend to be slightly smaller (by $\lesssim 10\%$) than those of Sternheimer.[6] The equations of the present paper are obviously valid for any reasonable choice of I values. By means of the density ρ_0, one obtains the plasma energy $h\nu_p$ [Eq. (5)]. From the values of I and $h\nu_p$, the parameter C [Eq. (3)], and hence the resulting X_a [Eq. (8)] are determined.

The use of the single exponent $m = 3.0$ and the resulting equation for a [Eq. (51)] imply that the cubic density effect term $a(X_1 - X)^3$ will be present for all substances, and hence the energy-loss formulas for dE/dx, $(dE/dx)_{W_0}$, and ϵ_{prob} can be written in a simple form, with the square bracket F being expressed as $F = F_1 - F_2$ [Eq. (56)], where $F_2 = a(X_1 - X)^3$.

We have given the formulas for F_1 in Sec. III, and Sec. IV of the paper contains a detailed discussion of two illustrative examples, which show how the various parameters (I, $h\nu_p$, A, B, C, a, m, X_0, X_1) are determined. The first example, namely, the calculation of δ for methane (CH_4) at $P = 20$ atm and $T = 20$ °C, illustrates the use of Eqs. (44)–(50) to obtain $\delta_\eta(p)$ pertaining to a density $\eta \rho_0$, where ρ_0 is the density of the gas at NTP. The second example concerns the calculation of the most probably energy loss ϵ_{prob} (as a function of $\gamma = E/m_0c^2$) in a sample of tungsten of thickness $t = 10$ g/cm^2.

In connection with the density effect, we note that a very comprehensive review of the theory and experiments on the density effect has been recently presented by Crispin and Fowler.[23] We also note that a review of the expressions for the ionization loss and of the experimental verification of the density effect (up to 1960) has been given by Sternheimer.[24]

Finally, we wish to mention three recent experiments which were especially designed to test the energy-loss formula (and hence the density effect) at extremely high energies. These experiments were carried out by Bellamy *et al.*[25] [energy loss and straggling of high-energy muons (up to $\gamma \sim 100$) in a NaI(Tl) crystal]; by Aitken *et al.*[26] [energy loss and straggling in silicon by high-energy electrons, π^+ mesons, and protons (up to $\gamma \sim 1500$)]; and by McNulty and Congel[27] (restricted energy loss of e^-, e^+, p, and π^+ in nuclear emulsion). All three experiments gave an excellent confirmation of the accuracy of the Bethe-Bloch formula, corrected for the density effect, up to the highest energies investigated, i.e., up to $\gamma \sim 8000$ for the experiment of McNulty and Congel.[27] These experiments thus provide no evidence for the reduction in energy loss at very high energies due to radiative corrections, which was predicted by Tsytovich.[28] A theoretical explanation for the absence of any appreciable ($\gtrsim 1\%$) reduction in energy loss has been given in Ref. 23.

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Electric-Field-Gradient Calculations in the Aluminum Silicates (Al_2SiO_5)[†]

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The point-multipole model is used to calculate the electric-field-gradient tensors at the eight nonequivalent aluminum sites of the three Al_2SiO_5 polymorphs, kyanite (four sites), andalusite (two sites), and sillimanite (two sites). The contribution from induced dipole and quadrupole moments of the oxygen ions is included. The oxygen-ion polarizabilities and the Al^{3+} Sternheimer factor are considered as variable parameters to fit NMR measurements of the 34 independent field-gradient components. The best fit (average disagreement 21%) is obtained with $\alpha_D = 0.5$ Å^3, $\alpha_Q = 0.1$ Å^5, and $\gamma_\infty = -4.9$. The disagreement is roughly the same at all eight sites. With the theoretical $\gamma_\infty = -2.4$, and $\alpha_D = 1.1$ Å^3, $\alpha_Q = 0.1$ Å^5, the disagreement is 21% at the six octahedral sites but 82% at the five-coordinated site in andalusite, and 103% at the tetrahedral site in sillimanite. The oxygen-dipole contribution is very large; the quadrupole contribution is generally small but not negligible. Two recent refinements of the kyanite structure enable errors due to inaccuracy in the crystal structure parameters to be estimated. The thermal vibrations of the ions determined by x rays are calculated, and their contribution to the field gradients found to be quite small.

I. INTRODUCTION

The ionic, or point-ion model, has frequently been used for the computation of electric field gradients in predominantly ionic crystals.[1–10] This model represents the charge distribution of a crystal by point multipoles fixed at the lattice sites. Given the crystal structure and the multipole polarizabilities of the ions, the potential distribution can be calculated by summation over the lattice. Field gradients computed in this manner can be compared with values derived from nuclear-quadrupole tensors eQV^n_{ij}/h at nuclear sites. Here Q is the nuclear-quadrupole moment and V^n_{ij} is the field-gradient tensor at the nucleus. V^n_{ij} is usually related to the calculated external field gradient V_{ij} by the Sternheimer antishielding factor[11] γ_∞, i.e., $V^n_{ij} = (1-\gamma_\infty)V_{ij}$. There often is considerable disagreement between the calculated and measured electric field gradients. This disagreement is usually ascribed to effects of the finite charge distribution of the negative ion, overlap, charge transfer, covalent bonding, etc. In other words, the disagreement is due to the approximations inherent in the ionic model. But in order to make an estimate of the importance of nonionic effects, it is first necessary to minimize errors in application of the ionic model. These are due to uncertainties in the atomic coordinates and the multipole polarizabilities of the ions. In comparing the theoretical field gradients with experiment results, uncertainties in the nuclear-quadrupole moment and the Sternheimer antishielding factor must be considered. Thermal vibrations of the ions must also be taken into account.[10]

Theoretical calculations are available for the multipole polarizabilities and γ_∞ for free ions, but their values for ions in a crystal cannot be predicted with any accuracy. The best approach is to study a crystal of low symmetry, so that there are a number of field-gradient components. Then the polarizabilities and γ_∞ can be used as variable parameters to fit the observed nuclear-quadrupole coupling data. It has been shown[2,3,8,10,12–14] that the multipole series must include at least the dipole and quadrupole terms. The effects of induced quadrupoles are more often than not ignored. When they have been considered, it has been for crystals[2,3,8,12–14] with too few field-gradient components to use the variable-parameter approach unambiguously. In only one case[10] ($AlPO_4$) has there been more than one parameter available for comparison.

The crystals with which this paper deals, kyanite,