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Comparison of exact and approximate formulas for the Mott correction to energy loss of relativistic heavy ions

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A comparison is given between an exact numerical calculation and two approximate analytic expressions for the Mott correction to energy loss of heavy ions. A complete tabulation of the Mott correction is given for use when the approximate expressions are not valid. The validity of possible relativistic corrections to the Bloch correction is discussed. A comparison of the calculations to some recent experiments is given.

I. INTRODUCTION

Corrections to the traditional Bethe formula for energy loss of heavy ions are of interest to experimental nuclear physics and cosmic ray physics. Any corrections which are not proportional to Z^2 where Z is the atomic number of the ion are of particular importance since Z^2 scaling is used in many experimental particle identification techniques. Bohr's original classical energy loss expression contained a term proportional to $Z^2 \ln Z$ and this was reconciled with Bethe's formula by Bloch's calculation[1] which reduces to Bethe's formula for $\alpha/\beta \ll 1$ (α/Z=fine-structure constant, β=velocity of ion/c) and to Bohr's formula when $\alpha/\beta \gg 1$. In the relativistic case, the fact that the cross section for Coulomb scattering of electrons (the Mott cross section) is not proportional to Z^2 leads to an additional non-Z^2 correction to energy loss. This Mott correction was first calculated by Eby and Morgan[2,3] numerically and several approximate analytical expressions have been proposed[3,4] for this correction. Ahlen[5] then redid Bloch's original calculation with some modifications and concluded that in addition to the nonrelativistic Bloch correction and the Mott correction there is a relativistic Bloch correction which depends on an undetermined parameter θ_0. Recently, Anderson *et al.*[6] have done a calculation based on a method of Cox, Golovchenko, and Goland[7] and this reproduces both the Bloch and Mott corrections exactly without any relativistic Bloch correction. The method of Ref. 6 permits a greatly simplified calculation of the Mott correction, reducing the problem to the numerical summation of an infinite series, rather than the extensive numerical integration required in Refs. 1 and 2.

This paper presents a complete tabulation of the Mott correction which is now feasible due to the simplified method of Anderson *et al.* It also gives a comparison of some of the approximate expressions for the Mott correction due to Ahlen[4] and Morgan and Eby[3] to the exact formula so that the range of validity of these approximate expressions can be accurately determined. A discussion of the relation of the method of Anderson *et al.* to Bloch's original calculation as redone by Ahlen is also given as well as a discussion of Ahlen's relativistic Bloch correction. Results of a recent experiment with relativistic gold ions are compared with the calculation.

II. THEORY

The contribution to energy loss from close collisions in which electron binding energy can be neglected is given by

$$dE/dX = N\int_{\eta}^{T_{\max}} dT(T\,d\sigma/dT)\ , \tag{1}$$

where η is an energy above which electron binding energy can be neglected, $d\sigma/dT$ is the cross section for energy loss, $T_{\max}=2mc^2\beta^2/(1-\beta^2)$ is the maximum energy transfer to an electron of mass m, βc is the incident ion velocity, and N is the number of electrons per unit volume of absorber. Using the relation between the energy transfer T and the center-of-mass scattering angle θ, $T=T_{\max}\sin^2(\theta/2)$, we have

$$\frac{dE}{dX} = N\pi T_{\max}\int_{\theta_0}^{\pi} d\theta\,\sin\theta(1-\cos\theta)(d\sigma/d\Omega)\ , \tag{2}$$

where $d\sigma/d\Omega$ is the electron-scattering cross section in the rest frame of the ion and θ_0 is the c.m. scattering angle corresponding to η. The Mott correction as originally defined[3] is given by

$$\Phi_m = \frac{\pi T_{\max}}{\xi}\int_{\theta_0}^{\pi} d\theta\,\sin\theta(1-\cos\theta) \times\left[\left(\frac{d\sigma}{d\Omega}\right)_{\rm Mott} - \left(\frac{d\sigma}{d\Omega}\right)_{\rm FB}\right]\ , \tag{3}$$

where $\xi=2\pi Z^2e^4/mv^2$ and $(d\sigma/d\Omega)_{\rm FB}$ is the first Born approximation expression for $(d\sigma/d\Omega)_{\rm Mott}$. This was originally calculated in Refs. 2 and 3 by computing $(d\sigma/d\Omega)_{\rm Mott}$ numerically and then performing the integral numerically. The numerical calculation of $(d\sigma/d\Omega)_{\rm Mott}$ was further used to evaluate the response of particle detectors which do not respond directly to dE/dX such as emulsions, ion chambers, and Cherenkov detectors.[8,9] Andersen *et al.*[5] pointed out that the integral in the expression for Φ_m can be done analytically in the limit $\theta_0 \to 0$. That is, if we take the phase shift expression for $(d\sigma/d\Omega)_{\rm Mott}$ and $(d\sigma/d\Omega)_{\rm FB}$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\rm Mott}=\frac{1}{4K^2}\left\{\left|\sum_{l=0}^{\infty}[(2l+1)(e^{2i\delta_l}-1)+l(e^{2i\delta_{-l-1}}-e^{2i\delta_l})P_l(\theta)]\right|^2+\left|\sum_{l=0}^{\infty}(e^{2i\delta_{-l-1}}-e^{2i\delta_l})P_l^1(\theta)\right|^2\right\}, \tag{4}$$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\rm FB}=\frac{Z^2e^4(1-\beta^2)}{4m^2v^4\sin^4(\theta/2)}[1-\beta^2\sin^2(\theta/2)] \tag{5}$$

$$\equiv\left[\frac{d\sigma}{d\Omega}\right]_R[1-\beta^2\sin^2(\theta/2)], \tag{6}$$

where

$$\left[\frac{d\sigma}{d\Omega}\right]_R=\frac{1}{4K^2}\left|\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_{l,0}}-1)P_l(\theta)\right|^2 \tag{7}$$

and

$$e^{2i\delta_l}=-\frac{l+1+i\alpha'/\beta}{\rho_l+1+i\alpha/\beta}\frac{\Gamma(\rho_{l+1}-i\alpha/\beta)}{\Gamma(\rho_{l+1}+i\alpha/\beta)}e^{-i\pi(\rho_{l+1}-l)},$$
$$e^{2i\delta_{-l-1}}=\frac{l-i\alpha'/\beta}{\rho_l-i\alpha/\beta}\frac{\Gamma(\rho_l+1-i\alpha/\beta)}{\Gamma(\rho_l+1+i\alpha/\beta)}e^{-i\pi(\rho_l-l)}, \tag{8}$$
$$e^{2i\delta_{l,0}}=\frac{\Gamma(l+1-i\alpha/\beta)}{\Gamma(l+1+i\alpha/\beta)},$$

where P_l^m are associated Legendre functions, δ_l,δ_{-l} are the Coulomb field expressions for the phase shifts, $v=\beta c$,

$$\hbar K=\frac{cm\beta}{(1-\beta^2)^{1/2}},\quad \alpha=Ze^2/\hbar c,$$

$$\gamma=\frac{1}{(1-\beta^2)^{1/2}},\quad \alpha'=\alpha/\gamma,$$

and $\rho_l=(l^2-\alpha^2)^{1/2}$, then the integrals can be done using standard relations for integrals of Legendre functions. The result is[6]

$$\Phi_m/2=\frac{\beta^2}{2}+\frac{\beta^2}{2\alpha^2}\sum_{l=0}^{\infty}\left[(l+1)\frac{[(l+1)^2-(\alpha/\beta)^2]}{[(l+1)^2+(\alpha/\beta)^2]}\frac{(l+1)}{(2l+1)(2l+3)}\frac{(l+1)^2-(\alpha'/\beta)^2}{[(l+1)^2+(\alpha'/\beta)^2]}\right.$$
$$\left.-\frac{(l+1)(l+2)}{(2l+3)}{\rm Re}(e^{2i(\delta_l-\delta_{l+1})})-\frac{l(l+1)}{2l+1}{\rm Re}(e^{2i(\delta_{-l-1}-\delta_{-l-2})})\right], \tag{9}$$

where the second term in $d\sigma/d\Omega_{\rm FB}$ directly gives the $+\beta^2/2$ term. This series can be summed numerically and produces results which agree with previous calculations in the cases where results are available. The approximate forms of Φ_m which have been suggested are

$$\Phi_1=\pi\alpha\beta+\alpha^2\left[\frac{\pi^2}{3}+1+\beta^2[\pi^2(\tfrac{3}{4}-\ln 2)-0.8990]\right],$$

$$\Phi_2=(\alpha\beta)(1.725+0.52\cos\chi)+\alpha^2(3.246-0.451\beta^2)+\alpha^3(1.522\beta+0.987/\beta)$$
$$+\alpha^4(4.569-0.494\beta^2-2.696/\beta^2)+\alpha^5(1.254\beta+0.222/\beta-1.170/\beta^3),$$

$$\cos\chi={\rm Re}\left[\frac{\Gamma(\tfrac{1}{2}-i\alpha/\beta)\Gamma(1+i\alpha/\beta)}{\Gamma(\tfrac{1}{2}+i\alpha/\beta)\Gamma(1-i\alpha/\beta)}\right],$$

where Φ_1 is due to Morgan and Eby[3] and Φ_2 to Ahlen.[10]

Φ_m can be computed by a different method by noting that $d\sigma/d\Omega_{\rm FB}$ in Eq. (5) can be obtained by letting $\rho_l=l$ in Eq. 4 for all β. When Eq. (4) is then used in Eq. (3), we find

$$\Phi_m'/2=\frac{\beta^2}{2\alpha^2}\sum_{l=0}^{\infty}-\frac{(l+1)(l+2)}{2l+3}{\rm Re}(e^{2i(\delta_l-\delta_{l+1})}-e^{2i(\delta_l-\delta_{l+1})}|_{\rho_l=l})$$
$$-\frac{l(l+1)}{2l+1}{\rm Re}(e^{2i(\delta_{-l-1}-\delta_{-l-2})}-e^{2i(\delta_{-l-1}-\delta_{-l-2})}|_{\rho_l=l}),$$

where the second term in each set of parentheses is evaluated for $\rho_l = l$. This expression can be calculated in two ways. We can use the same numerical method to calculate the first and second term in both brackets or we can use the analytical expressions for the second terms in each bracket as given by Eqs. (8). The result of this latter procedure is

$$\Phi''_m/2 = \frac{\beta^2}{2\alpha^2} \sum_{l=0}^{\infty} -\frac{(l+1)(l+2)}{(2l+3)} \mathrm{Re}(e^{2i(\delta_l - \delta_{l+1}')}) - \frac{l(l+1)}{2l+1} \mathrm{Re}(e^{2i(\delta_{-l-1} - \delta_{-l-2}')})$$

$$+ \frac{(l+1)(l+2)}{2l+3} \frac{[(l+1)^2 - \alpha\alpha'/\beta^2][(l+2)^2 + \alpha\alpha'/\beta^2] - (l+1)(l+2)\left[\dfrac{\alpha^2 - (\alpha')^2}{\beta^2}\right]}{[(l+1)^2 + (\alpha/\beta)^2][(l+2)^2 + (\alpha'/\beta)^2]}$$

$$+ \frac{l(l+1)}{2l+1} \frac{(l^2 + \alpha\alpha'/\beta^2)[(l+1)^2 - \alpha\alpha'/\beta^2] - l(l+1)\left[\dfrac{\alpha^2 - (\alpha')^2}{\beta^2}\right]}{[l^2 + (\alpha/\beta)^2][(l+1)^2 + (\alpha'/\beta)^2]} .$$

Both of these alternate expressions have been computed and give good argument with Eq. (9) except for the absence of the term $\beta^2/2$. This is because the second term in Eq. (6) gives a finite contribution to Eq. (3) in the limit $\theta_0 \to 0$ while the first term in Eq. (6) gives an infinite contribution in Eq. (3) in the limit $\theta_0 \to 0$ and only results in a finite number when subtracted from the $d\sigma/d\Omega_{\mathrm{Mott}}$ terms in Eq. (3). In this subtraction of two infinite terms in the limit $\theta_0 \to 0$, the finite $\beta^2/2$ term is apparently lost. However, both $\Phi'_m/2 + \beta^2/2$ and $\Phi''_m/2 + \beta^2/2$ give good agreement with $\Phi_m/2$ and also with the approximate expression for $\Phi_1/2$ and $\Phi_2/2$ in their region of validity. This gives us an additional check of the numerical accuracy in the calculation.

To calculate the total dE/dX, Ref. 6 used a trick suggested by Lindhard and used by Cox, Golovchenko, and Goland.[7] If the phase shift expression for $d\sigma/d\Omega_R$ is used in Eq. (2), then in the limit $\theta_0 \to 0$ the integral can be done analytically but it diverges. One then truncates the series in l at an $l_{\max}$ such that the collision duration equals a characteristic orbit time and obtains the usual nonrelativistic Bethe formula plus the complete Bloch correction, which arises from relatively small l values so that the series for the Bloch correction does not need to be truncated. In the relativistic case, the procedure of Ref. 6 can be made more explicit in the following way. If we assume that there is a correspondence between l and the impact parameter b such that

$$\hbar l = m\gamma v b ,$$

then truncating the series in Eq. (2) corresponds to limiting the collisions to impact parameters less than $b_0 = \hbar l_{\max}/m\gamma v$. This can then be joined to distant collision expressions such as those of Ahlen.[5] Specifically, if $d\sigma/d\Omega_R$ in Eq. (7) is substituted in Eq. (2) and the integrals done in the limit $\theta_0 \to 0$ we have, following Ref. 7, for large $l_{\max}$

$$dE/dX_R = 2N\xi(\ln l_{\max} + \Phi_B)$$

$$= 2N\xi\left[\ln\left[\frac{\gamma m v b_0}{\hbar}\right] + \Phi_B\right] ,$$

where

$$\Phi_B = \frac{-\alpha^2}{\beta^2} \sum_{l=0}^{\infty} \frac{1}{[(l+1)^2 + (\alpha/\beta)^2](l+1)} .$$

Combining this with Ahlen's formula for distant collisions[5] (see also Jackson[11])

$$dE/dX_D = 2N\xi\left[\ln\left[\frac{(1.123)\gamma v}{b_0\langle w\rangle}\right] - \beta^2/2\right]$$

and defining the empirically determined average ionization potential I by

$$I = 2\frac{\hbar\langle w\rangle}{1.123}$$

we find

$$\frac{dE}{dX} = \frac{dE}{dX_D} + \frac{dE}{dX_R} + N\xi(\Phi_m - \beta^2)$$

$$= 2N\xi\left[\ln\left[\frac{2mv^2\gamma^2}{I}\right] - \beta^2 + \Phi_m/2 + \Phi_B\right] \quad (10)$$

as in Ref. 6. A term in $\ln\gamma$ and $-\beta^2/2$ comes from both distant and close collisions as it should. This type of approximation should be valid as long as $l_{\max}$ is large and thus $\hbar/mv\gamma b_0$ is small.

Ahlen's relativistic Bloch correction contains the parameter θ_0. It is based on the third Born approximation wave functions for the range of $\theta < \theta_0$ which gives rise to the Bloch correction. If θ_0 is taken sufficiently small then the relativistic Bloch correction is negligible and Ahlen's calculation agrees with Eq. (10). On the other hand, if the result depends on θ_0 then Bloch's procedure of joining results from the three regimes would seem to break down.

III. RESULTS

Figs. 1–8 show a comparison of Φ_m, Φ_1, and Φ_2 for a range of Z and β. Φ_1 is a better approximation to Φ_m for low Z and moderate β than Φ_2. For large Z and moderate β, however, Φ_2 is the better approximation. Both approximations begin to fail for $Z/\beta \gtrsim 100$ as is clear from Figs. 1 and 2. This is as expected as is stated

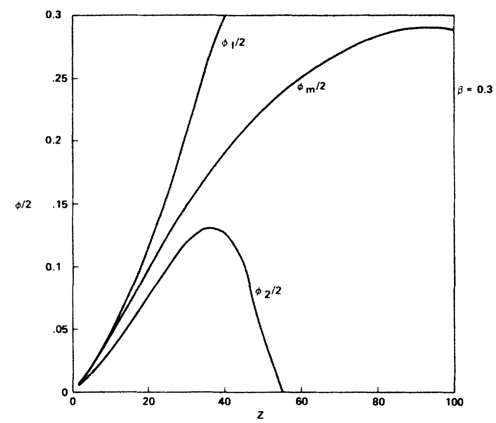

FIG. 1. Φ vs Z for $\beta=0.3$.

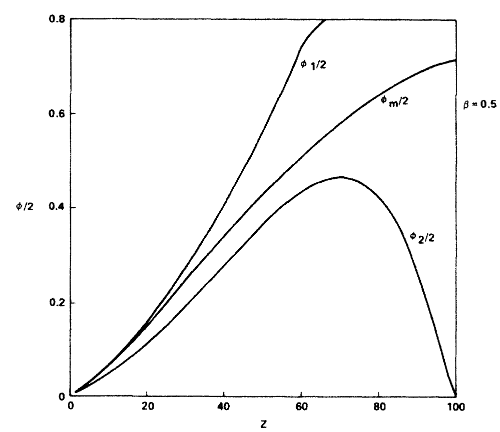

FIG. 2. Φ vs Z for $\beta=0.5$.

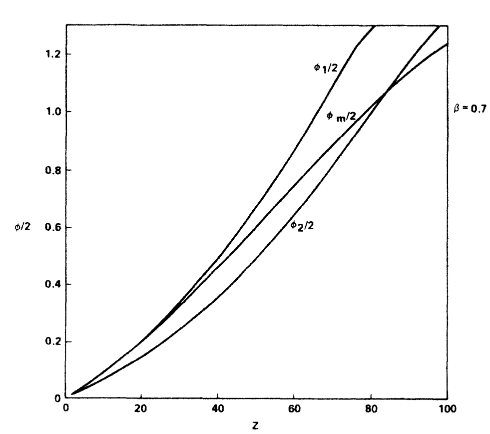

FIG. 3. Φ vs Z for $\beta=0.7$.

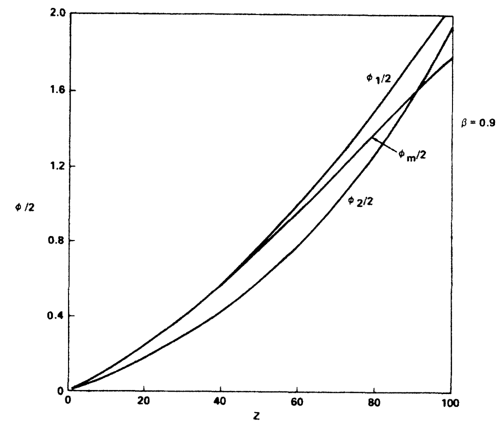

FIG. 4. Φ vs Z for $\beta=0.9$.

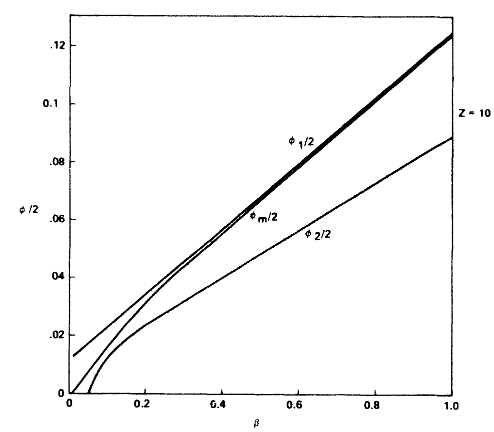

FIG. 5. Φ vs β for $Z=10$.

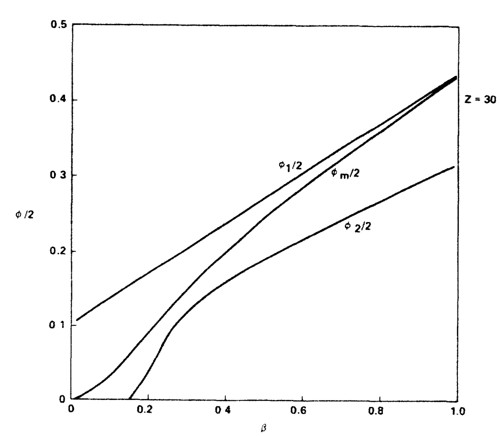

FIG. 6. Φ vs β for $Z=30$.

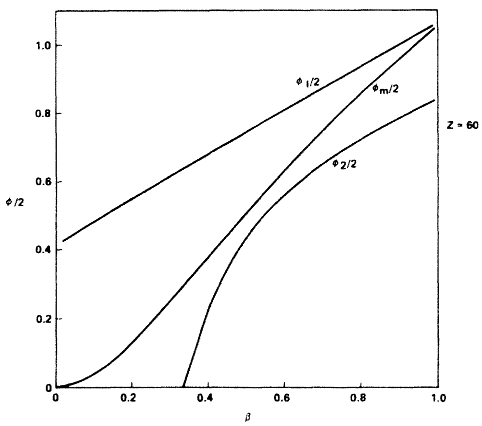

FIG. 7. Φ vs β for $Z=60$.

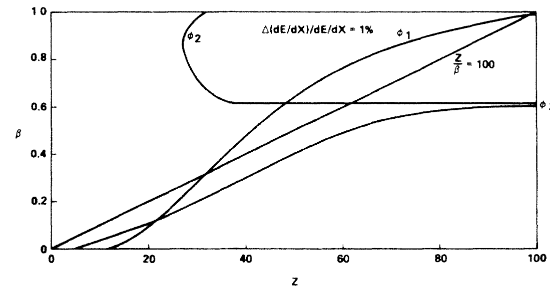

FIG. 9. Values of Z and β for which use of Φ_1 and Φ_2 give an energy loss which differs by 1% from that computed using Φ_m.

in Ref. 4. This is further illustrated in Fig. 9 where the values of Z and β, for which the error in dE/dX from Eq. (10) due to the use of Φ_1 or Φ_2 instead of Φ_m, is 1%. We see this occurs in the regions of $Z/\beta \sim 100$. For the cases in which Φ_1 and Φ_2 are not good approximations we have included a tabulation of $\Phi_m/2$ in Table I. This table includes values of Φ_m for lower values of β than have previously been tabulated. The simplified numerical method described here makes these calculations feasible in this regime. The expressions for $\Phi_m'/2+\beta^2/2$ and $\Phi_m''/2+\beta^2/2$ give nearly the same values as in Table I. They are both typically smaller than $\Phi_m/2$ by several percent but agree with each other to a five figure accuracy. This gives a further check on the accuracy of the calculation. Several hundred terms in the series for Φ_m gives about a three significant figure accuracy.

This tabulation of Φ_m should be useful in dE/dX calculations and especially in range correction calculations where one must follow the slowing ion to low β. A misuse of Φ_2 outside its region of validity will give incorrect range values since Φ_2 becomes large and negative for low β as seen from the figures.

Figure 10 shows the results of an experimental calibration of the HEAO-3 Heavy Cosmic Ray Experiment ion chambers at the Bevalac (Ref. 14) using a relativistic $_{25}$Mn and $_{79}$Au beam. Previous calculations of energy deposit[9] show that energy loss is nearly equal to energy deposit for the energies used in the experiment. The figure indicates that our calculation with the Mott correction only is in better agreement with the data than the Mott + Bloch corrections. We have also calculated Ahlen's relativistic Bloch correction (referred to as C_R in Ref. 5) for three values of the parameter θ_0. For $\theta_0=0.01$, C_R has a negligible effect on the calculation and the curve for Mott + Bloch + C_R coincides with that of Mott + Bloch corrections. For $\theta_0=0.1$, C_R nearly cancels the Mott and Bloch correction and the data for $_{79}$Au correspond to the data for $_{25}$Mn, i.e., essentially no non-Z^2 effect. For $\theta_0=0.05$, C_R reduces the Mott + Bloch curve as shown in the figure. The theoretical Mn curve is normalized to 1 at 1 GeV/nuc, i.e., it gives the ratio of $(dE/dX_{\rm Mn})^{1/2}$ to $[dE/dX_{\rm Mn}(E=1\ {\rm GeV/nuc})]^{1/2}$. The theoretical Au curve is the ratio of $\frac{25}{79}(dE/dX_{\rm Au})^{1/2}$ to the quantity $[dE/dX_{\rm Mn}(E=1\ {\rm GeV/nuc}\ )]^{1/2}$. The experimental Mn

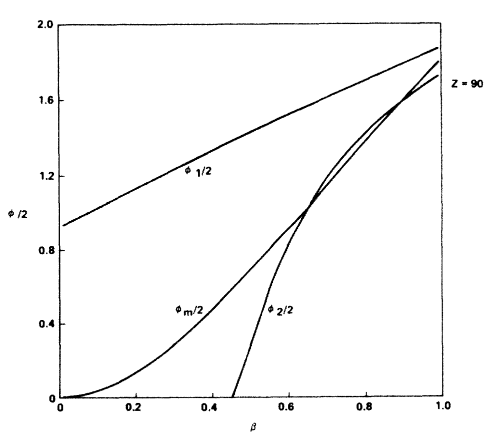

FIG. 8. Φ vs β for $Z=90$.

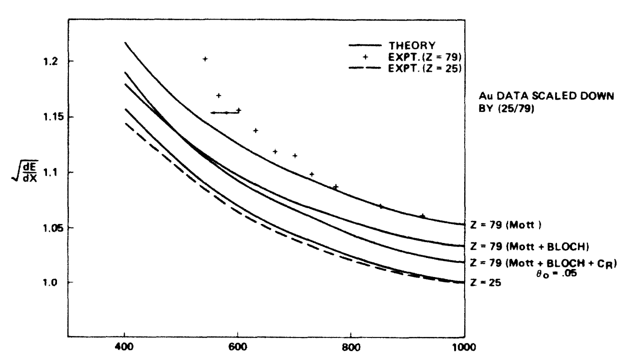

FIG. 10. Ion chamber response from an experiment using $_{25}$Mn and $_{79}$Au compared with theory. The Au data are scaled down by a factor of $\frac{25}{79}$. The absorber was a 90% argon $-$10% methane mixture (by partial pressure) for which $I=191$ eV was used.

TABLE I. Mott correction to energy loss ($\Phi_m/2$).

β \ Z	1	10	20	30	40	50	60	70	80	90	100
0.01	0.0001	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0003
0.1	0.001	0.016	0.027	0.033	0.036	0.037	0.038	0.038	0.038	0.037	0.035
0.2	0.002	0.031	0.066	0.092	0.110	0.123	0.132	0.137	0.140	0.139	0.136
0.3	0.004	0.044	0.098	0.150	0.192	0.225	0.252	0.272	0.286	0.292	0.291
0.4	0.005	0.056	0.127	0.201	0.270	0.331	0.383	0.426	0.459	0.481	0.490
0.5	0.006	0.068	0.153	0.247	0.341	0.432	0.514	0.586	0.647	0.694	0.723
0.6	0.007	0.079	0.177	0.289	0.407	0.525	0.639	0.745	0.841	0.921	0.979
0.7	0.008	0.091	0.202	0.329	0.467	0.611	0.756	0.899	1.03	1.15	1.25
0.8	0.009	0.102	0.225	0.367	0.523	0.691	0.866	1.04	1.21	1.38	1.53
0.9	0.011	0.114	0.249	0.403	0.577	0.766	0.968	1.18	1.39	1.61	1.81
0.99	0.012	0.125	0.270	0.436	0.624	0.831	1.05	1.30	1.55	1.81	2.06

curve is the ratio of $(I_{\rm Mn})^{1/2}$ to the quantity $[I_{\rm Mn}(E=1\ {\rm GeV/nuc})]^{1/2}$ taken directly from Ref. 14. The experimental Au points are the ratio of $\frac{25}{79}(I_{\rm Au})^{1/2}$ to the quantity $[I_{\rm Mn}(E=1\ {\rm GeV/nuc})]^{1/2}$ from Ref. 14 where I is the ion chamber output. The lower energies in the figure were obtained by placing absorbers in the beam and calculating the energy loss using a computer program which included the relativistic Bloch correction. Our calculations indicate that the difference in dE/dX (Mott) and dE/dX (Mott + Bloch + C_R) for $\theta_0=0.1$ amounts to about 12% in this energy range for $Z=79$. Use of the Mott correction only would shift the data points to the left for Au relative to the initial energy of 1009 MeV/nuc. For example, the point at 600 MeV would be shifted to the left by about 50 MeV giving better agreement with the upper theoretical curve in Fig. 10. If the Mott + Bloch correction is used, the corresponding difference between dE/dX (Mott + Bloch) and dE/dX (Mott + Bloch + C_R) is about 6% in this energy range for $Z=79$. The double arrows in the figure indicate how the data would be shifted for these possibilities. Errors in the initial energy determination of the Au or Mn beam would shift the upper experimental curve horizontally relative to the lower one, possibly improving the agreement with theory.

We do not believe that this data provides a definitive test of the validity of the Mott, Bloch, and relativistic Bloch corrections. Comparison of dE/dX with ion chamber output requires two assumptions: (i) Energy deposit is equal to energy loss and (ii) ion chamber response is proportional to energy deposit. We believe the first assumption is valid in this experimental situation because of the detailed calculations for the identical detector configuration given in Ref. 9. The second assumption has yet to be tested in this energy and charge region. It is possible that the Bloch and relativistic Bloch corrections are present in the energy-loss corrections but not in the ion chamber response. The high-energy delta rays for which the Mott correction is largest will definitely contribute to ion chamber output if they do not escape from the ion chamber (and this effect is accounted for in the calculations of Ref. 9 for the data considered here). For the Bloch corrections, which are quantum-mechanical effects related to the construction of a wave packet in the original Bloch calculation, it is less clear how these might affect ion chamber output. A definitive test of these higher-order energy-loss corrections would require a direct measurement of particle energy (e.g., by using a magnetic field) before and after traversing suitable absorber material for a range of energies and charges. The kind of experimental comparison described here may aid in the development of models of ion chamber response which could improve detector charge resolution in experiments such as the HEAO experiment discussed here.

IV. CONCLUSION

We have shown that the validity of the two approximate expressions for the Mott correction is restricted to $Z/\beta \lesssim 100$ for a 1% accuracy in dE/dX, as expected. When this condition is not satisfied, we have given a tabulation of the Mott correction which should be of use both in accelerator and cosmic ray experiments involving heavy ions. In particular, these tables can be used in range calculations applicable to experiments such as those of Ahlen and Tarle,[12] Waddington *et al.*,[15] and Waddington *et al.*[13] The first two of these indicated an agreement with the Mott + Bloch + C_R corrections to range while the third was consistent with the Mott + Bloch corrections as described here.

We have shown that the HEAO-3 detector calibration gives better agreement with the theory if the Mott correction only is used than if either the Mott and Bloch or Mott, Bloch, and relativistic Bloch corrections are used. This may be useful for constructing models of ion chamber response for relativistic heavy nuclei.

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