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# Shell correction for the stopping power of K electrons

P.T. Leung
*Portland State University*

M. L. Rustgi

S. A. Long



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# Shell correction for the stopping power of $K$ electrons

P. T. Leung* and M. L. Rustgi
*Physics Department, State University of New York at Buffalo, Buffalo, New York 14260*

S. A. T. Long
*Langley Research Center, National Aeronautics and Space Administration, Hampton, Virginia 23865*
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In view of the inapplicability of the asymptotic expressions for the stopping number available in the literature at high energies, an alternative approach is taken to compute the shell correction to the stopping number of $K$ electrons. Anholt's formula for the $K$-shell ionization has been used to calculate the excitation function for longitudinal interaction and numerical integration over energy has been carried out to evaluate the shell correction. Comparison with other theoretical calculations is made. It is proposed that, with the inclusion of relativistic effects, an asymptotic expansion of the stopping number with a leading-term logarithmic in the energy of the incident particle would be more meaningful and might enable one to extract the relativistic contribution to the shell correction from it.

## INTRODUCTION

The evaluation of the shell corrections to the Bethe formula for the stopping power of matter has remained an active area of research ever since the pioneering work of Bethe and collaborators in the early 1950's.[1-5] By considering the optical oscillator strength and the mean excitation energy of the target atom, they were able to obtain some asymptotic formulas for the shellwise stopping number ($B_i$) for various target elements using screened hydrogenic orbitals. The shell correction ($C_i$) could then be extracted from a comparison made between the exact $B_i$ obtained from numerical integration and the asymptotic $B_i$ so obtained. The results of this approach have been reviewed in the literature by Uehling and Fano.[6,7] Developments along this line have been carried on by Khandelwal[8] to cover the entire Periodic Table for the $K$ and $L$ shells which have the most important contributions to shell corrections and, quite recently, improved asymptotic formulas have been obtained using Hartree-Slater oscillator strengths by Khandelwal.[9] Aside from this line of development, recently there have been different approaches attempted by others such as the extraction of $C_K$ and $C_L$ from explicit Born-approximation calculations on subshell stopping powers by McGuire[10] and the kinetic theoretical description by Sabin and Oddershede[11] based on Sigmund's formalism.[12] In spite of all these, Walske's results[4,5] have many times been regarded as references for comparison between "hydrogenic calculations" with experimental or other theoretical results.[10-14] It is the purpose of this paper to point out that due to the nonrelativistic nature, the asymptotic formulas given in the literature are not applicable for high-incident energies and hence the calculation of the shell correction by exploiting these formulas may not have general validity. Furthermore, it will be desirable to include the relativistic nature of the $K$ electrons for heavy elements. We have therefore in this work followed an alternative approach to integrate the shell correction numerically and the results are compared with those from other theoretical investigations. We shall limit ourselves only to the $K$ shell contribution ($C_K$) in this paper and always take proton as the incident particle.

## THE STOPPING NUMBERS

The asymptotic formulas of Walske[4] and Khandelwal[8,9] can be summarized as follows. The stopping number $B_K$ is expanded in inverse power of the incident particle's velocity as follows:[1-3]

$$B_K(\theta_K,\eta_K)=S_K(\theta_K)\ln\eta_K+T_K(\theta_K)-C_K(\theta_K,\eta_K) \tag{1}$$

with

$$C_K(\theta_K,\eta_K)=U_K(\theta_K)\eta_K^{-1}+V_K(\theta_K)\eta_K^{-2}+\cdots . \tag{2}$$

In (1) and (2), $\theta_K$ is the screening parameter which increases with the atomic number of the target atom and $\eta_K=v^2/Z_K^2$ with $v$ being the incident particle's velocity and $Z_K=Z-0.3$ the effective charge of the target atom. The coefficients $S_K$, $T_K$, $U_K$, and $V_K$ are listed in Refs. 8 and 9 and we have used everything in atomic units in this paper. Because of the nonrelativistic nature of both the incident particle and the $K$ electrons assumed in deriving these formulas, the results are not applicable in the limit of very large $\eta_K$'s corresponding to high incident energies or in the case with heavy target elements. For high-energy incident protons, it is more suitable to express $\eta_K$ in the form

$$\left[\frac{137}{Z_K}\right]^2\left[1-\left[\frac{0.938}{E_p}\right]^2\right]$$

as explained later on with $E_p$ being the energy of the proton in GeV.

 

While $B_K$ can be described by the asymptotic form using Eq. (1), it can also be obtained by exact integration. In the first Born approximation and by considering only the direct Coulomb interaction (i.e., only the longitudinal photon effect), $B_K$ can be written as

$$B_K(\theta_K,\eta_K)=\int_{W_{\min}}^{\infty} dW \int_{Q_{\min}}^{\infty} dQ \frac{1}{Q}\phi_W(Q) , \tag{3}$$

with

$$\phi_W(Q)=\frac{W|F_W(Q)|^2}{Q} , \tag{4}$$

where $F_W(Q)$ is the inelastic Coulomb form factor for the excitations and ionization of the target atom. $W$ and $Q$ are the energy and momentum transfers in atomic units. From kinematics and conservation of energy and momentum, one can set $W_{\min}=\theta_K$ and $Q_{\min}=W^2/4\eta_K$.[15] For hydrogenlike wave functions, $|F_W(Q)|^2$ has the following form according to Anholt:[16]

$$|F_W(Q)|^2=\frac{2^7 d^2}{3}(3Q+W)Q\frac{\exp\left[-\frac{2}{k}\tan^{-1}[2k/(Q+1-k^2)]\right]}{[1-\exp(-2\pi/k)][(Q-k^2+1)^2+4k^2]^3} , \tag{5}$$

where

$$k^2=W-1 , \tag{6}$$

and

$$d^2=\left[1+\left[\frac{Z_K\alpha}{2}\right]^2\right]^{-1}\left[1+(W-1)\left[\frac{Z_K\alpha}{2}\right]^2\right]^{-1} \tag{7}$$

arises from the normalization constants since we have used semirelativistic Darwin wave functions to describe the atomic $K$ electron. Similar but somewhat different expressions have also been obtained by Davidović *et al.*[17] but since Anholt's results agree better with experiment, we have here adopted his formalism. Previous formulations using Schrödinger wave functions would be equivalent to the above results by setting $d^2=1$.[1-5] $\alpha$ in Eq. (7) stands for the fine-structure constant. Numerical integration for Eq. (3) has been carried out for various elements using a $256\times256$ points Gaussian quadrature for all energies. At low energies, our results reproduce the previous results if we set $d^2=1$.[4,8] At higher energies, where the asymptotic formulas of Walske and Khandelwal are not valid, our exactly integrated results for $B_K$ with and without the effect of $d^2$ are shown in Fig. 1. It is clear from this figure that the use of the Darwin wave function gives very different results from those using the Schrödinger wave function for target elements with a large $Z$, since the $K$ electrons of the heavy atoms are quite relativistic in nature. In fact, Anholt had pointed out earlier[16] that the tables published previously[8,18] have to be modified due to the inclusion of the factor $d^2$, although for light elements such as carbon there is essentially no difference with or without the $d^2$ term. However, for light elements, $\eta_K$ becomes very large at large incident energies and hence Eqs. (1) and (2) cannot be applied. Taking into consideration this fact and the effect of the $d^2$ term, we conclude that the previous $C_K$'s calculated from Eqs. (1) and (2) are of questionable accuracy for high-incident energies for both light and heavy target elements. Furthermore, it is also worthwhile to point out that the expansion formulas for $B_K$ given in the literature lose their asymptotic nature completely once the relativistic nature of the $K$ electrons is taken into taken into account (the $d^2$ factor) as shown in Fig. 2. In the following, therefore, we attempt to recompute $C_K$ including the $d^2$ term by following an alternative method originally suggested in Walske's paper.[4]

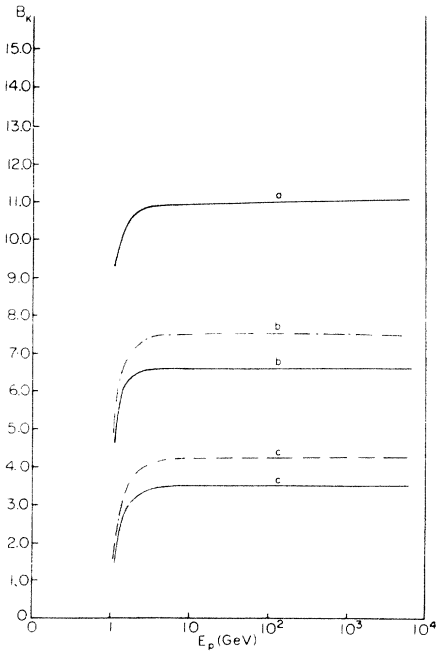


FIG. 1. Stopping number $B_K$ and the effect of $d^2$ on it. The solid line represents the exact results of this work and the dash-dotted line represents the integrated result without the factor $d^2$. The curve labeled $a$ is for $C$ ($\theta_K=0.64$) with the range of $\eta_K$ being $60<\eta_K<600$; the integrated results with or without $d^2$ almost overlap with each other. The curve $b$ is for Ni ($\theta_K=0.8$) with the range of $\eta_K$ being $5<\eta_K<25$ and the curve $c$ is for Pm ($\theta_K=0.9$) with the range of $\eta_K$ being $1<\eta_K<5.5$.

## CALCULATION OF $C_K$

Bethe, Brown, and Walske[2] have considered the following function:

$$X(\theta_K,\eta_K)=\int_0^\infty dW\int_{1/4\eta_K}^{4\eta_K}dQ\frac{1}{Q}\phi_W(Q)-\int_{W_m}^\infty dW\int_{1/4\eta_K}^{W^2/4\eta_K}dQ\frac{1}{Q}\phi_W(0)$$
$$-\lim_{Q_1\to 0}\int_0^{W_m}dW\int_{1/4\eta_K}^{Q_1}dQ\frac{1}{Q}\phi_W(0)-\lim_{Q_1\to 0}\int_0^{W_m}dW\int_{Q_1}^\infty dQ\frac{1}{Q}\phi_W(Q) \tag{8}$$

and have shown that $X\sim A\ln_K+B$ for all $\eta_K$ and fixed $\theta_K$. Hence by comparing (1) and (8), one can find $C_K$ as

$$-C_K=B_K-X\ . \tag{9}$$

In what follows, we shall first rederive Eq. (8) of Ref. 4 in a bit simpler way than the original one and then apply numerical integration techniques to compute $C_K$ from Eq. (9).

The first integral of Eq. (8) can be rewritten as

$$\int_0^\infty dW\int_{1/4\eta_K}^{4\eta_K}dQ\frac{1}{Q}\phi_W(Q)=\int_{W_m}^\infty dW\int_{1/4\eta_K}^{4\eta_K}dQ\frac{1}{Q}\phi_W(Q)$$
$$+\int_0^{W_m}dW\int_{1/4\eta_K}^{0}dQ\frac{1}{Q}\phi_W(Q)+\int_0^{W_m}dW\int_0^{4\eta_K}dQ\frac{1}{Q}\phi_W(Q)\ . \tag{10}$$

Substitute (10) into (8), recombine terms and we can write

$$X(\theta_K,\eta_K)=\int_{W_m}^\infty dW\int_{1/4\eta_K}^{4\eta_K}dQ\frac{1}{Q}\phi_W(Q)-\int_{W_m}^0 dW\int_{1/4\eta_K}^{W^2/4\eta_K}dQ\frac{1}{Q}\phi_W(0)+\int_0^{W_m}dW\int_{1/4\eta_K}^0 dQ\frac{1}{Q}[\phi_W(Q)-\phi_w(0)]$$
$$-\int_0^{W_m}dw\int_{4\eta_K}^\infty dQ\frac{1}{Q}\phi_W(Q)\ . \tag{11}$$

Substituting (3) and (11) into (9), we get

$$-C_K=\int_{W_m}^\infty dW\int_{W^2/4\eta_K}^\infty dQ\frac{1}{Q}\phi_W(Q)-\int_{W_m}^\infty dW\int_{1/4\eta_K}^{4\eta_K}dQ\frac{1}{Q}\phi_W(Q)+\int_{W_m}^\infty dW\int_{1/4\eta_K}^{W^2/4\eta_K}dQ\frac{1}{Q}\phi_W(0)$$
$$+\int_0^{W_m}dW\int_{4\eta_K}^\infty dQ\frac{1}{Q}\phi_W(Q)+\int_0^{W_m}dW\int_0^{1/4\eta_K}dQ\frac{1}{Q}[\phi_W(Q)-\phi_W(0)]\ . \tag{12}$$

Let us denote the last integral by $C'$ and rewrite it as follows:

$$C'=\int_0^\infty dW\int_0^{1/4\eta_K}dQ\frac{1}{Q}[\phi_W(Q)-\phi_W(0)]-\int_{W_m}^\infty dW\int_0^{1/4\eta_K}dQ\frac{1}{Q}[\phi_W(Q)-\phi_W(0)]\ . \tag{13}$$

Interchanging the order of integration in the first term in (13) and applying the Bethe sum rule[19] in the form

$$\int_0^\infty dW\,\phi_W(Q)=\int_0^\infty dW\,\phi_W(0)\ , \tag{14}$$

we get only the second term left for $C'$. Substituting back in (12) and neglecting the fourth term in (12) because it becomes less than $10^{-2}$ for $\eta_K\gtrsim 0.5$, one obtains

$$-C_K=\int_{W_m}^\infty dW\int_{W^2/4\eta_K}^\infty dQ\frac{1}{Q}\phi_W(Q)-\int_{W_m}^\infty dW\int_{1/4\eta_K}^{4\eta_K}dQ\frac{1}{Q}\phi_W(Q)+\int_{W_m}^\infty dW\int_{1/4\eta_K}^{W^2/4\eta_K}dW\frac{1}{Q}\phi_W(0)$$
$$-\int_{W_m}^\infty dW\int_0^{1/4\eta_K}dQ\frac{1}{Q}[\phi_W(Q)-\phi_W(0)]\ . \tag{15}$$

If we rewrite the last term in (15) as

$$-\int_{W_m}^\infty dW\int_0^{W^2/4\eta_K}dQ\frac{1}{Q}[\phi_W(Q)-\phi_W(0)]-\int_{W_m}^\infty dW\int_{W^2/4\eta_K}^{1/4\eta_K}dQ\frac{1}{Q}\phi_W(Q)+\int_{W_m}^\infty dW\int_{W^2/4\eta_K}^{1/4\eta_K}dQ\frac{1}{Q}\phi_W(0)\ , \tag{16}$$

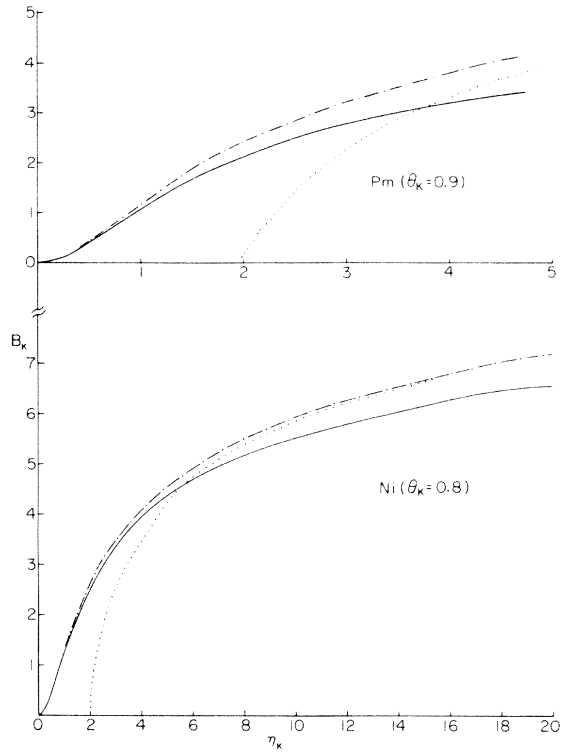


FIG. 2. Comparison of the integrated results for $B_K$ with the asymptotic formulas given in Ref. 8. The solid line represents the exact result with the factor $d^2$. The dash-dotted line represents the integrated result without the factor $d^2$ and the dotted line represents the results of the asymptotic formulas.

substitute (16) back in (15), simplify and regroup terms, we arrive finally at Eq. (8) of Ref. (4),

$$-C_K=\int_{W_m}^{\infty}dW\int_{4\eta_K}^{\infty}dQ\frac{1}{Q}\phi_W(Q)-\int_{W_m}^{\infty}dW\int_0^{W^2/4\eta_K}dQ\frac{1}{Q}[\phi_W(Q)-\phi_W(0)]\,. \tag{17}$$

Note that we have only applied the sum rule once in our derivation. With the $\phi_W(Q)$ being given above [Eqs. (4)—(7)], we have computed $C_K$ via numerical integration for various elements. Incidentally, we found that it is more convenient to manipulate with the four integrals in Eq. (15) than the two in Eq. (17) because of faster convergence and above all, the first term in Eq. (15) is just the $B_K$ which we have computed before and the third term is independent of $\eta_K$. In Fig. 3 we show a comparison of the results obtained in this work and Walske's original results for two elements: Ni ($\theta_K=0.8$) and Pm ($\theta_K=0.9$). Figure 4 shows a comparison between the present result with the results from other calculations.[4,10,11]

## DISCUSSION AND CONCLUSION

It is seen in Fig. 3 that the results obtained in this work are in general smaller than those of Walske's original calculations. Furthermore, the results here seem to show a reverse trend as far as the screening parameter ($\theta_K$) is concerned. In fact, it will be very interesting if one can argue physically what the trend of the $C_K$ should be with respect to the variation of atomic number of the target element. It should also be remarked that the curves in Fig. 3 are trustworthy only for not too high values of $\eta_K$ since the expansion of $C_K$ in $O(1/\eta_K)$ will never vanish since $\eta_K$ approaches a maximum value as the velocity of the incident particle approaches that of light, whereas we expect that no shell correction is necessary for incident particles with infinitely high energies.[20] We suggest the lower limit $0.2\leq 1/\eta_K$ for the $C_K$ curves to be trustworthy. Furthermore, since the Bethe sum rule [Eq. (14)] holds exactly only for nonrelativistic atomic wave functions while we have been using Darwin wave functions in our formalism, the results for heavy target element (e.g., for $\theta_K=0.9$) will not be very accurate. However, since the term $d^2$ does not play an important role for light atoms (see Fig. 1), we expect that our results for Ni ($\theta_K=0.8$) and Al ($\theta_K=0.7$) would still be quite accurate.

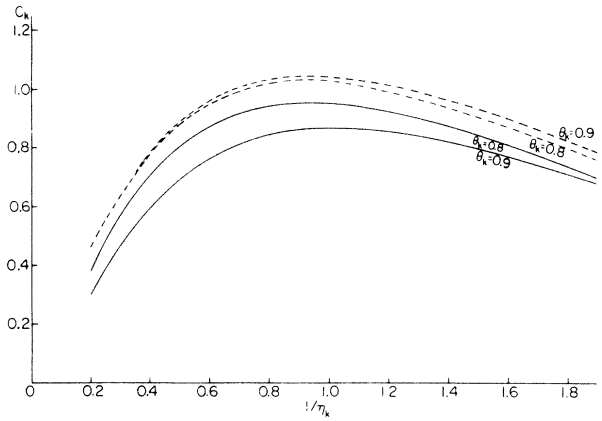


FIG. 3. Comparison between this work and that of Walske (Ref. 4) for $C_k$. The solid line represents the results of the present work and the dashed line represents Walske's results.

The comparison of $C_K$ for Al from different calculations is shown in Fig. 4. It is interesting to note that

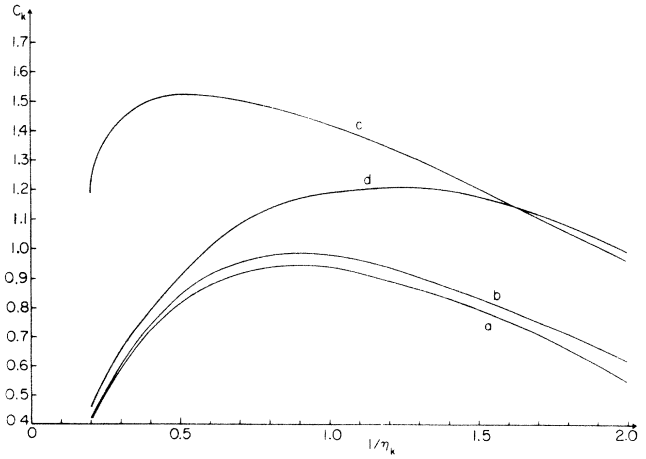


FIG. 4. Comparison of $C_K$ for Al from different theoretical calculations. *a* is the result of this work, *b* is Walske's results (Ref. 4), *c* is the result of McGuire (Ref. 10), and *d* is the result of Sabin and Oddershede (Ref. 11).

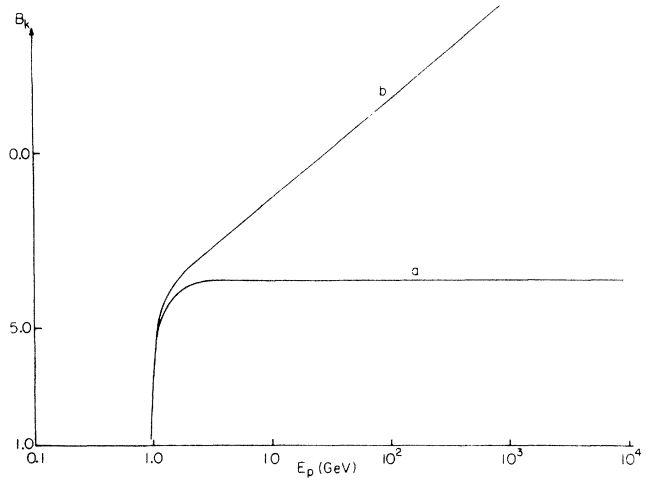


FIG. 5. Stopping number for Ni. *a* includes only longitudinal effect and *b* includes the sum of longitudinal, transverse, and spin-flip effect.

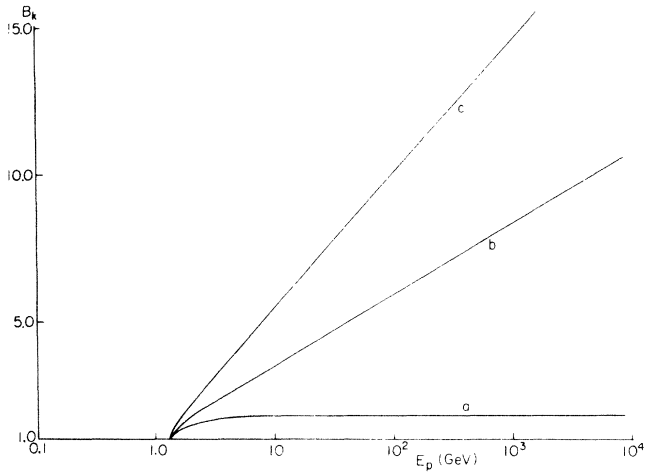


FIG. 6. Stopping number for *U*. *a* includes only longitudinal effect, *b* includes the sum of longitudinal and transverse effects, and *c* includes the sum of longitudinal, transverse, and spin-flip effects.

while the present result is quite close to Walske's original result, both results are consistently smaller than the result of McGuire.[10] It may be more interesting to note that the result of Sabin and Oddershede[11] lies just between the two results mentioned above, being very close to the "hydrogenic results" for high-incident energies and very close to McGuire's result for low-incident energies. It would be of great interest if we can understand more physically the behaviors of these various results. Finally, it might also be of interest if one can find new asymptotic formulas for $B_K$ which better fit the exact integrated results in Fig. 1 and reproduce the $C_K$ curves in Fig. 4 at the same time.

However, from previous investigations[21] the "saturation characteristics" of the $B_K$'s will disappear if we also include the relativistic effects, namely, the transverse and spin-flip effects.[16,17] Figures 5 and 6 show the results for Ni and U from which we can see the importance of the spin-flip effect for heavy elements. Furthermore, it is found that with the inclusion of relativistic effects, $B_K$ becomes almost linear in $\ln(E_p)$ and hence we propose that it might be more meaningful to seek asymptotic expansion of $B_K$ with a leading logarithmic term in energy (rather than in velocity) of the incident particle. In other words, $\eta_K$ should be defined to be proportional to energy only if all these other relativistic effects are included. In that case, we might be able to extract the shell correction accurately for all energies with the relativistic effects (mainly the spin-flip effect for heavy target atoms) on $C_K$ being included. Of course, one is always left with the possibility that other processes (e.g., pair creation in the atomic field of the target) may come in which suppress the $B_K$ curve again towards saturation at high-incident energies so that an expansion in velocity ($\sim\eta_K$) with modified coefficients may still be possible. All these will be left as a future study in the relativistic effects on the shell corrections of Bethe's theory of stopping power of matter.

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*Permanent address: Physics Department, Tamkang University, Tansui, Taiwan 251, Republic of China.

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