

# Stopping power, $Z_1^3$ – Parameter, Bloch and Shell Corrections in Bethe Formula for Protons and Helium Ions in DNA and Liquid Water

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## Abstract

The Barkas effect happen because of target electrons due to responding to the approaching particle and slightly changing the orbits before occur from interaction of energy loss (denominate target polarization). At high energies (above  $20v_0 \approx 10MeV/u$ ) insignificant because the ion moving too fast to cause initial motion the target electrons where at low energies  $\ll 1 MeV/u$  the Barkas effect is investigated.

**Keywords:** Barkas effect, energy loss, Stopping power, and Beth - Bloch equation.

## الخلاصة

أن تأثير باركز الحاصل بسبب الكترولونات الهدف واستجابة لأقتراب جسيم وما يسببه من تغيير طفيف للمدارات وذلك قبل حدوث تفاعل فقدان الطاقة ( يدعى بأستقطاب الهدف ) عند الطاقات العالية (فوق  $20v_0 \approx 10MeV/u$ ) تأثير باركز ليس ذات أهمية بسبب حركة الأيون السريعة جدا والمسببة حركة ابتدائية للكترولونات الهدف بينما في الطاقات الواطنة الأقل من  $1 MeV/u$  يظهر تأثير باركز.

## Introduction

Energy loss theory of fast charged particles in matter is based on the calculations by Bethe [1], who derived the stopping power in the first Born approximation. The Bethe result is proportional to the projectiles charge squared,  $Z_1^2$ . Barkas *et al.* [2] found that the range of negative pions is longer than positive pions of equal momentum, therefore, Barkas *et al.* [3] suggested that the effect is due to a difference in the stopping power determined from the opposite charge of the projectiles. The reduction in the stopping power, responsible for the longer range of negatively charged particles as compared to their positively charged antiparticles was later investigated with sigma hyperons [3], pions [4], and muons [5], but these measurements all suffered from the inferior quality of the low velocity particles and antiparticles beams used. This is called Barkas effect which, interpreted as a polarization effect in the stopping material, depending on the charge of the projectile. It seems as the second term (proportional to  $Z_1^3$ )

in the implied born expansion of the energy loss. Barkas effect for interaction of protons and Helium ions with Deoxyribonucleic acid (DNA) and liquid water has been studied and calculated in present work using Bragg's rule. A program is written in Fortran-90 for numerical calculations.

In present work stopping power, Barkas effects, Bloch and shell corrections have been investigated for the interaction of protons and Helium ions in Deoxyribonucleic acid (DNA) ( $C_{20}H_{27}N_7O_{13}P_2$ ) and liquid water. Bragg's rule has been used on each element in DNA and liquid water to determine the parameters correction in Bethe-Bloch formula using Ziegler's semi-empirical formula.

## Materials and Methodology

The basic stopping equation for particles with high velocity is given as [6]:

$$-\frac{1}{\rho} \frac{dE}{d\ell} = 3.0705 \times 10^{-4} \frac{Z_1^2 Z_2}{A_2 \beta^2} L, \quad (1)$$

Where  $-\frac{1}{\rho} \frac{dE}{d\ell}$  is in ( $MeV.cm^2 / mg$ ); L is the stopping number;  $Z_1, Z_2$  are the atomic numbers of incident ions and target ;  $A_2$  and  $\rho$  are the atomic mass and density of target ;  $\beta = v/c$  , where  $v$  and  $c$  are the incident ion velocity and speed of light.

The unit of equation (1) for stopping cross-section S, transform in units,

$$S(ev.cm^2 \times 10^{-15}/atom)$$

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$$= 1.6605A_2 \left[ 3.0705 \times 10^{-4} \frac{Z_1^2 Z_2}{A_2 \beta^2} L \right]$$

$$= (4.928 \times 10^{-4} \frac{Z_1^2 Z_2}{\beta^2}) L \quad (2)$$

The stopping number L, defined to include the correction clause to the stopping equation, and can be defined as an expansion in powers of the atomic number Z of the particle:[6],

$$L(\beta) = L_0(\beta) + Z_1 L_1(\beta) + Z_1^2 L_2(\beta) \quad (3)$$

Where:

$L_0(\beta)$  Born Correction;  $Z_1 L_1(\beta)$  Barkas effect Correction;  $Z_1^2 L_2(\beta)$  Bloch corrections:

$$L_0(\beta) = \log\left(\frac{2mv^2}{I}\right) - \left(\frac{C}{Z_2}\right), \quad (4)$$

Where  $\left(-\frac{C}{Z_2}\right)$  is the shell correction term.

Take some special cases:

(i) For incident proton, with  $Z_1=1$ ,

$$L_P = L_0 + L_1 + (L_2)_P \quad (5a)$$

(ii) For incident Helium ion, with  $Z_1=2$ ,

$$L_{He} = L_0 + 2L_1 + (L_2)_{He} \quad (5b)$$

Therefore:

$$L_1 = L_P \left(\frac{L_{He}}{L_P} - 1\right) + (L_2)_P - (L_2)_{He} \quad (6)$$

Practical value of Barkas effect  $(L_1)_{exp}$  determined from the relative difference  $\Delta$  of stopping power for both proton and helium.

Where  $\Delta = 1 - \frac{4S_P}{S_{He}}$ ,  $(7a)$

Substituting equation (2) in (7a) for  $S_P$  and  $S_{He}$  one can get,

$$\Delta = 1 - \frac{L_P}{L_{He}}, \quad (7b)$$

Rewriting equation (7b) in the following form:

$$\frac{L_{He}}{L_P} = \frac{1}{1 - \Delta},$$

$$\frac{L_{He}}{L_P} - 1 = \frac{1}{1 - \Delta} - 1 = \frac{1 - (1 - \Delta)}{1 - \Delta} = \frac{\Delta}{1 - \Delta} \quad (8)$$

If  $\Delta \ll 1$ , then

$$(1 - \Delta)^{-1} \approx (1 + \Delta),$$

Therefore, equation (8) becomes:

$$\frac{L_{He}}{L_P} - 1 \cong \Delta(1 + \Delta) \quad (9)$$

Substituting equation (9) into equation (6) for  $\left(\frac{L_{He}}{L_P} - 1\right)$ , and will get

$$L_1 = L_P \Delta(1 + \Delta) + (L_2)_P - (L_2)_{He} \quad (10)$$

From equation (10) one can determine the Barkas effect.

According to the Bloch correction definition [7]:

$$(Z_1^2 L_2) = -1.202y^2 + 1.037y^4 - 1.008y^2 \quad (11)$$

Where  $y = Z_1^2 v_0^2 / v^2$

From equations (3 and 4) one can calculates Bloch correction and Barkas effects and therefore according to equation. (5) The shell correction is either,

$$\left(-\frac{C}{Z_2}\right) = L_{He} - \log(2mv^2/I) - (L_1)_{He} - (L_2)_{He}, \quad (12a)$$

or

$$\left(-\frac{C}{Z_2}\right) = L_P - \log(2mv^2/I) - (L_1)_P - (L_2)_P, \quad (12b)$$

Using Bragg's rule to determine stopping power of compounds [8]:

$$S(A_m B_n) = mS(A) + nS(B) \quad (13)$$

Where  $S(B), S(A)$  are the stopping powers for A, B in unit  $ev.cm^2 \times 10^{-15}/atom$ ,  $n, m$ : Are the numbers of atoms to elements A, B in particle of compounds.

From Beth -Bloch equation the stopping number  $L_{exp}$  is as follows:

$$L_{exp} = \frac{\beta^2}{KZ_1^2} S_{exp} \quad (14)$$

Where  $S_{exp}$  is the stopping power from SRIM software 2003 [9], therefore using equations (7,10,11 and 12) together with equations.(13

and 14) one can find Barkas effects, Bloch correction and shell correction depending on the Stopping and Range of Ions in Matter (SRIM) output.

### Results and Discussion

Figure 1 shows the stopping cross-section,  $S$ , in  $(eV.cm^2 \times 10^{-15} / atom)$  for hydrogen and helium ions in liquid water ( $H_2O$ ) with incident ion energy  $E(MeV / amu)$ . The maximum value of stopping cross-section for Helium ions is approximately twice than for Hydrogen ion i.e.  $(S_{He} / S_H) \approx 2$  at energy  $E(MeV / amu) = 0.0225$  and  $0.225$  for liquid water as shown in Figure 1.

Figure 2 shows the stopping cross-section,  $S$ , in  $(eV.cm^2 \times 10^{-15} / atom)$  for hydrogen and helium ions in DNA ( $C_{20}H_{27}N_7O_{13}P_2$ ) with incident ion energy  $E(MeV / amu)$ . The maximum value of stopping cross-section for Helium ions is approximately twice than for Hydrogen ion i.e.  $(S_{He} / S_H) \approx 2$  at energy  $E(MeV / amu) = 0.0225$  and  $0.225$  for DNA and comparison between pervious work and present work as shown in Figure 2.

Figure 3 shows the variation of Barkas effect  $L_1$  with incident ion energy  $E$  (MeV/amu). The first note is that  $L_1$  is independent of incident ions atomic number  $Z_1$  as shown in figure, and the other thing: at low energy  $E \approx 0.01(MeV / amu)$   $L_1 \approx 50$  and  $0.65$  for liquid water and DNA. Also for liquid water  $L_1$  decreases as ion energy increases while for DNA the behavior is completely different, also Barkas effect  $L_1$  is going to zero a  $E(MeV / amu) \geq 0.1$  for liquid water and  $-0.2 > L_1 > 0$  for DNA. Figure 4 shell correction  $(-C/Z_2)$  for proton and the He-ions in liquid water,  $H_2O$  and DNA is shown in Figures (4a and 4b). There is no significant

difference in shell correction  $(-C/Z_2)$  for proton or He-ions in liquid water ,its maximum value  $\approx -85$  at energy  $E \leq 0.1$  MeV/u and approach to zero at  $E \geq 0.1$  as shown in Figure (4a), while the shell correction  $(-C/Z_2)$  for DNA is about  $8.5$  at  $E \leq 0.1$  and nearly equal to zero at  $E \geq 0.1$  ,as shown in Figure (4b). We can say that the maximum value of  $(-C/Z_2)_{H_2O} \approx 10 (-C/Z_2)_{DNA}$  as shown in Figure (4a, 4b) and  $(-C/Z_2) \rightarrow 0$  at  $E \geq 0.1$ .

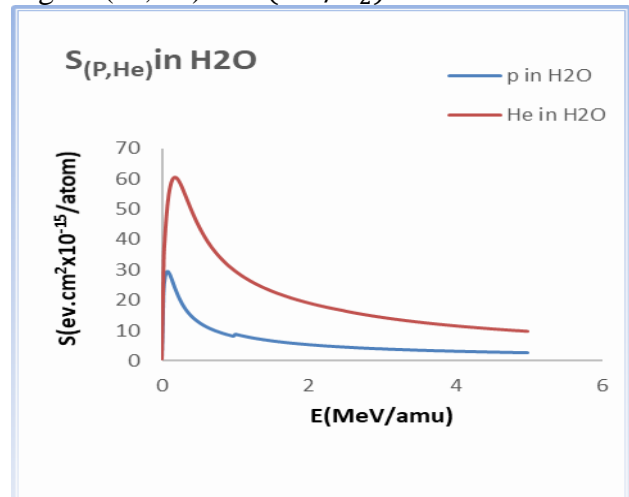


Figure 1: Stopping cross section  $S$  in  $(eV.cm^2 \times 10^{-15} / atom)$  of H and He ions in liquid water with incident ion energy  $E$  in (MeV/amu).

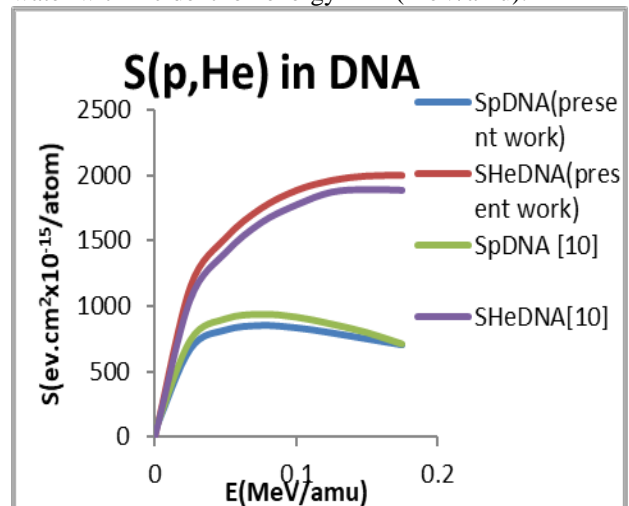


Figure 2: Stopping cross section  $S$  in  $(eV.cm^2 \times 10^{-15} / atom)$  of H and He ions in DNA with incident ion energy  $E$  in (MeV/amu) and comparison between present work and previous work [10].

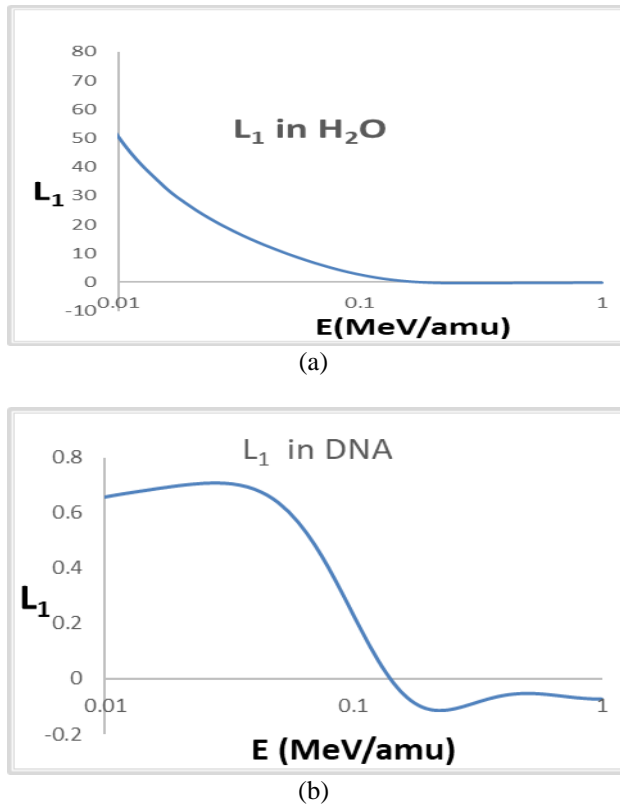


Figure 3: Barks effect  $L_1$  for proton and Helium in (a) liquid water and (b) in DNA with incident ion energy  $E$  in (MeV/amu).

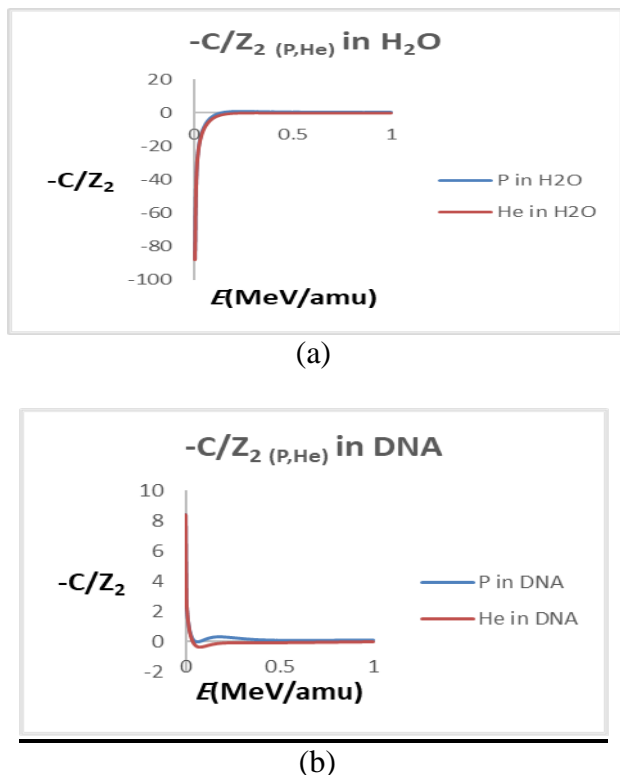


Figure 4: Shell correction ( $-C/Z_2$ ) in (a) for proton and He-ion in liquid water and (b) in DNA with incident ion energy  $E$  in (MeV/amu).

### Conclusions

in present work Beth-Bloch formula used as Ziegler's semi-empirical to investigate the interaction between Proton and Helium ions in water and DNA then calculated stopping power, Bloch and shell corrections for proton and Helium together with SRIM (Stopping and Range of Ions in Matter) software 2003 program output. The maximum value of stopping cross-section for Helium ions twice than for proton ions in liquid water and DNA and Barkas effect is independent of incident ions atomic number. At low energy Barkas effect,  $L_1 \approx 50$  for liquid water and 0.65 for DNA but when energy for incident ion increase Barks effect for liquid water decrease while for DNA this effect is completely different. There is no significant difference in shell correction for proton or He-ions in liquid water we can say that the maximum value of shell correction for liquid water approximately tenth than for DNA.

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