Exact analytical solution of the lateral spread of a particle beam in matter  
within a nonsmall angle limit

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**Abstract**

This work is the construction of an analytical theory of lateral spread within a nonsmall angle limit of an ionic or atomic beam in a target medium. The exact angular distribution theory was developed by Goudsmit and Saunderson; however, exact lateral spread model has not been constructed. Recently, ion beam cancer therapy is widely studied. Thus, the author is motivated to make a lateral spread theory involving small to large scattering angles and including the energy loss effect. The present study is successfully performed using the Bessel function, and exact analytical and numerical results are given in this text. The present research is expected to be useful for particle beam cancer treatment.

*Keywords*: Lateral spread, nonsmall angle limit, Thomas–Fermi–Moliere potential

# INTRODUCTION

The present study treats a nonrelativistic energy ion beam that penetrates into an amorphous target matter. Each particle undergoes successions of elastic- and inelastic-scattering collisions. After these collisions, each particle in the beam changes its direction, resulting in beam spreading. For example, as one of expected applications of the present study, in a proton or heavy-ion beam therapy, the estimation of angular distribution and of lateral spread is needed because both are altered by collisions with the penetration depth. The energy in particle beam therapy is relativistic; however, as a basic study of interaction between particle and matter, relativistic effects are not considered in the present study. Transport equation is exactly solved in the present treatment.

A pioneering work of an angular distribution theory within a nonsmall angle limit was proposed by Goudsmit and Saunderson in the 1940s [ (1), (2)]. Furthermore, within a small angle limit, Sigmund, Winterbon, and Marwick created theories for angular and lateral distributions in the 1970s [ (3), (4)]. However, any lateral spread theory within nonsmall angle limit has not yet been developed. Recently, several experimental studies on carbon ion beam radiotherapy have been performed [ (5) (6) (7)]. These studies have stimulated some investigators in this field to develop a more exactly treated theory on the lateral spread of a particle beam within a nonsmall angle limit. In the previous study of Ikegami [ (8)], Goudsmit and Saunderson’s (GS) theory has been extended from a non-energy-loss effect model to energy loss effect model. The next step is the exact construction of a lateral spread theory within a nonsmall angle limit.

Thus, the present study has aimed at the development of a new lateral spread model, and has been very well performed using the Bessel functions. An exact solution of a transport equation for the lateral spread will be shown hereafter. In the framework of a small angle limit, Marwick and Sigmund (MS) developed a lateral spread theory in 1975 [ (4)]. The previous study of Ikegami [ (8) (9)] introduced very well both of elastic and inelastic energy loss effects into MS’s theory. The improved MS theory thus obtained is proper treatment for the energy loss effect within a small angle limit. Extent of the improved MS theory is , and the limit of MS theory must be . The symbols , and are the reduced target thickness, lateral spread and target thickness, respectively (see Eqs. (17) and (18)). Furthermore, Liang has constructed in the 1998 a formulation of lateral range straggling by taking both elastic and inelastic energy loss effects into account [ (10)]. The present theory involves the inelastic energy loss effect.

# THEORETICAL BACKGROUND

It would be helpful for readers to survey simply the development of theoretical studies of particle-beam scattering in solid matters. Following categories may be helpful to get hold of theoretical studies reported so far:

(a) calculation within small angle limit, or within non-small angle limit

(b) calculation of angular distribution, or of lateral spread, or of both

(c) calculation taking account of energy-loss effect, or not, and if taking, inelastic, or elastic, or both

(d) calculation using basic variables with dimension (like length, mass, charge, etc.) or using reduced variables with non-dimension

The reduced variables are non-dimensional variables that is defined in Eqs. (5, 17a, 17b, 18). The present theoretical study can be categorized as the non-small angle limit, the lateral spread and the reduced variables. Then previous papers coming under this category may be summarized simply as following way. Within small angle limit, Sigmund and Winterbon (SW) constructed the multiple scattering theory in 1974 [ (3)]. In 1975, MS [ (4)] developed a lateral spread theory within a small angle framework based on SW’s treatment. Furthermore, with the use of reduced variables, comparisons among different projectile–target combinations for SW’s and MS’s theories have became possible. Valdes and Arista (VA) improved SW’s theory in 1994 [ (11)] by introducing the inelastic energy loss effect into SW’s model. Ikegami developed in 2013 the modified VA theory by taking the elastic energy loss effect into account [ (9)].

As for the theory within non-small angle limit, the first theoretical study date back to 1940 when Gaudsmit and Saunderson derived so-called GS model [ (1) (2)]. Their model is useful for recent ion radiotherapy because wide-angle scattering is important for large-energy losses in the target matter. Moreover, Ikegami improved GS’s theory in 2017 [ (8)]. The GS–Ikegami theory involves elastic and inelastic energy loss effects.

# THEORY

The assumptions in the present study are as follows:

1. Target atoms are randomly and homogeneously distributed.
2. Inelastic energy loss effect in each collision is considered.
3. Each collision is only a binary collision with a target atom.
4. Elastic and inelastic collisions are considered.
5. Scaling property is held because of using the reduced variables.

The above assumptions are the same as those for the standard GS model [ (1) (2)] and almost the same as those for SW’s and MS’s models [ (3) (4)], except for the small angle limit in the latter two. Scaling property is derived by using the reduced variables that can provide a universal curve for numerical results. The present theory does not limit target thickness whether target is thick or thin, and the present treatment is involving not only small scattering angle but also large angle.

In the present investigation, the final goal is constructing Eq. (26). The ion beam initially goes along the x-axis in Fig. 1. The beam changes its direction by elastic collisions with the target atoms in the matter. The effect of inelastic collision is introduced in Eq. (20) by using VA treatment. The present lateral spread theory begins with a standard transport equation as follows:

(1a)

(1b)

where (*i* = 1,2) is the distribution function, and symbol) means non-dimensional parameters. The quantity is the penetration depth in a target film, and hence is the small penetration length in a target. In the right-hand side of Eq. (1a), the first term is the distribution with collision involving change in the lateral spread at the first angle (), and the second term is the distribution at the second angle () without any collisions (just passing through a matter). Then, after making in Eq. (1a), we obtain Eq. (1b). Here, is the lateral spread caused by single scattering.

Then parameters in Eqs (1a) and (1b) are described hereafter.

(2)

(3)

(4)

(5)

(6)

(7)

and

(8)

is the screening length of Lindhard et al. [ (12)], and is the differential scattering cross-section derived by Lindhard and co-workers [ (12)]. The non-dimensional cross section in Eq. (8), the non-dimensional penetration depth in Eq. (3), non-dimensional lateral spread (*i* = 1, 2) in Eq. (4), and the non-dimensional target atom density in Eq. (7) are introduced, respectively. The parameter is the target foil thickness, is the Bohr radius, (1, 2) is the lateral spread, (1, 2) is the path length, (1, 2) is the deflection angle, and are the reduced initial and the reduced final energies, and are the initial kinetic energy of projectile and the final kinetic energy of projectile, respectively. is the atomic number of the projectile, is the atomic number of the target, is the elementary charge, is the number density of the target atoms per unit volume.

The distribution function (*i* = 1,2) is expressed by the Bessel function as follows:

(9a)

(9b)

is the m-order Bessel function of the first kind. Moreover, we use the following relations:

(10)

, (11)

where

is the *l*–order Bessel function of first kind.

Using Eqs. (10) and (11) for Eqs. (2) and (3), we have the following equations:

(13)

and,

. (14)

Here, C in the relation (14) is the initial constant for normalization. The lateral spread function must be max at lateral spread = 0; thus, *l* must be 0. And then, *l* = 0 decides that *m* is 0. No summation on *l* and *m* is caused by analytical calculation process. We, consequently, regard and as 0.

The interatomic potential in this study is the Thomas–Fermi–Moliere potential. In accordance with Meyer’s treatment [ (13)], the maximum impact parameter is defined by half the distance of neighboring atoms as:

(15)

Moreover, in accordance with SW’s and MS’s treatment [ (3) (4)], new variables are introduced as in the following way because of mainly numerical reason as follows:

, (16)

where

, (17a)

, (17b)

, (18)

and

. (19)

The quantity is the reduced penetration depth, and is the reduced target thickness. The quantity is the reduced lateral spread, same as MS’s treatment. The quantity is the ratio of incident and out-going energy of projectiles.

The next step is introducing the energy loss effects in accordance with VA [ (11)] and Ikegami [ (9)]. The basic relations for this purpose contain inelastic energy loss. Hereafter, subscripts *e*, indicate quantities related to the inelastic energy-loss (stopping) region. At first, the inelastic energy loss part is given by (please see Ref. [ (8)]):

(20)

where

(21)

Eqs. (20) and (21) are the same of VA model [ (11)]. Then, the nondimensional integration variable , the reduced energy , and the scattering intensity parameter are given by:

(22)

(23)

and

, (24)

Here, *k* is the scattering angle parameter affected by a single collision, and is the same as those in the definition of Eq. (5). is the projectile initial energy. As Final result, the transport cross section Δ and the lateral spread function (final equation) redefined are given as following relations:

(25)

and

(26)

In Eqs. (25), and (26), defined by Eq. (27) is the ratios of incident and out-going energies (after passing through the target foil) for the inelastic energy loss. The quantity is the lateral spread at single collision. The parameter C is the normalized constant. The basic equations are obtained. This equation Eq. (26) is remarkable since it relates non-small angle lateral spreads in matter. Hereafter, additional explanations are mentioned for , scattering cross-section, and MS’ formula.

The quantity is described very briefly as (please see the detailed description in Ref. [ (9)]:

, (27)

where

, (28)

, (29)

, (30)

(31)

and

. (32)

Here, is the initial velocity of an incident atom, is the Bohr velocity, and is defined by the formula . The quantity is the mass of an electron. The quantity *n*e is the electron density in the target matter, is the number of free electrons per atom, *kF* is the Fermi wave number, is the Fermi velocity, and is a constant [(14)].

It should be mentioned that Lindhard’s scattering cross-section [ (12)]:

(33)

is valid with regard to large scattering angles,

(34)

(35)

Here, is the scattering function derived by Lindhard et al., is the mass of the projectile, is the mass of the target atom. The quantity is the angle in the center of the mass system (C.M.S.).

Moreover, if the projectile and the target atoms are the same, relation of angles between the laboratory system (L.S.) and C.M.S. is given by

(36)

and then,

(37)

Thus, we can calculate the scattering cross section as:

(38)

Here, is the angle in L.S.

For comparison the lateral spread equation of MS model is written by [ (4)]:

(39)

where

(40)

and

. (41)

# RESULTS AND DISCUSSION

In the present study, Fortran numerical code is written by the author, and a commercial subroutine code is used. In Figs. 2–3, show examples of calculations of the lateral spread function obtained in Eq. (26). Through all of the present figures, the collisional system calculated is for C–C; however, as a matter of fact, projectile and target are not limited to only C–C because scaling property is held by using the reduced variables. In principle, we can compare other combinations of projectile and target atoms, not only with that of C and C but also each other. In other words, the present numerical results cover any pair of collisional systems including the C–C system. Moreover, we can make comparison at any projectile energies of any collisional systems [ (3) (4) (8) (9) (11)]. This is the reason why the present results are shown by using the reduced variables. Moreover, elastic energy losses effect is neglected in the present study because of a numerical problem. The numerical problem is oscillation of Bessel function, thus intensity of particle distribution of lateral spread is not down in larger .

Figure 2 shows variation of the lateral spread for two values of the inelastic energy–loss ratio . The values of cited are 0.9 (10% energy loss), and 0.8 (20% energy loss). The incident energy is 30 keV, the reduced thickness is 0.1 (0.85 nm), and the scattering parameter *k* is 1. A larger provides broader curves. A large means a big energy loss. Although the present results obtained are natural, we find that the influence of on the lateral spread is markedly large.

Figure 3 shows the comparison of curves for three values of reduced target thickness: = 0.1 (0.85 nm), 0.15 (1.2 nm), and 0.2 (1.7 nm). The parameters adopted are *k* = 1, incident energy is 30 keV, and = 0.5. The present study gives calculation results that a larger provides broader lateral spreads. The number of collisions increases when the target thickness is larger. Thus, the results obtained are considered to be proper.

In the calculations shown in Figs. 2 and 3, the same value of the scattering parameter *k* was used. Appreciable effect *k* was not obtained. From a physical mathematics point of view, the *k* dependence (i.e., *z* dependence of Eq. (22)) is seen only in the transport cross section (Eq. (25)). Thus, *k* effect is very limited in the present model. This is the reason why *k* dependence was not considered in the present numerical calculations.

Figure 4 (a) shows the comparison of the present and the MS theoretical results with the experimental data [ (15)]. Collisional system is O on Xe. Incident energies are 50, 60, 100, and 120 keV, and the reduced target thickness is 0.162 (). The results of experiments and theories are normalized to the half width of . The scattering parameter *k* is 1.5. The present results seem to be appropriate in absolute values within the range below . However, we cannot show the numerical results for because of a numerical problem. The numerical problem is occurrence of oscillation that is caused from Bessel function properties. The present theory involves large scattering angles in comparison with the MS’s treatment within the small angle limit. In spite of this, the calculated result of the lateral spread reproduces very well the experimental results in the range below . In the range upper , we cut off numerical calculation because of numerical problem. Figure 4 (b) (c) show theoretical results with basic variable of in atomic unit. In Fig. 4 (b), the curve of 60 keV is slightly broader than 50 keV, and in Fig. 4 (c), the curve of 120 keV also is broader than 100 keV.

Figure 5 (a), (b), (c) and (d) show the theoretical curves for = 0.1 (), = 1, and collisional system is C on O (gaseous oxygen at density 1.4291 kg/m3). Parameters of Fig. 5 (a) are 1 MeV, and = 0.7, parameters of Fig. 5 (b) are 1 MeV, and = 0.3, parameters of Fig. 5 (c) are 10 MeV, and = 0.7, and parameters of Fig. 5 (d) are 10 MeV, and = 0.7. Figure 6 (a) and (b) show the theoretical curves for = 0.1 (), = 1, and collisional system C on H (gaseous hydrogen at density 0.0899 kg/m3). Parameters of Fig. 6 (a) are 10 MeV, and = 0.7, parameters of Fig. 6 (b) are 10 MeV, and = 0.3 The tails of each curve in Figs 5 (a, b, c, d) and 6 (a ,b) are lower, but not enough because of a numerical problem. The problem is oscillation of Bessel function.

Advantages of the present results are to involve large scattering angle and to include large energy loss, even though the present study has numerical problem. Small angle approximation means that scattering angle is less than 20, but the present treatment has no limit of angle. The present results drastically changed by the definitions of Eqs. (3, 4, 7, 8), and the future problem is to find more suitable definitions of variables.

# CONCLUSIONS AND REMARKS

In the present study, the theoretical development has been done of an exact analytical solution of lateral spread taking the inelastic energy loss effect into account in the present model. Moreover, the effects of , and in Figs. 1, and 2, are given, respectively. The present research is expected to be useful for the ion beam radiotherapy.

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**AUTHOR CONTRIBUTION STATEMENT**

The present investigation is performed by one researcher that is Seiji IKEGAMI. Other researcher do not contribute to this study.

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**Figure captions**

Fig. 1: Geometrical explanation of lateral spread. The initial projectile direction is along the x axis. After collision, angular deviation is and lateral spread is .

Fig. 2: Comparison of the numerical results of obtained for three values of . The parameters adopted are = 0.1 (0.85 nm); incident energy = 30 keV; and = 1. Solid, and dotted lines correspond to = 0.9 and 0.8, respectively. Vertical and horizontal axes are the normalized intensity and the lateral spread , respectively.

Fig. 3: Comparison of the numerical results of for three values of . The parameters adopted are = 0.5; incident energy = 30 keV; and = 1. Solid, broken, and dotted lines correspond to = 0.1 (0.85 nm), 0.15 (1.2 nm), and 0.2 (1.7 nm), respectively. Vertical and horizontal axes are the normalized intensity and the lateral spread , respectively.

Fig. 4: (a) Comparison between experiment and theories for the reduced target thickness is 0.162 (), incident energies are 50, 60, 100, and 120 keV, collisional system is O on Xe. Vertical and horizontal axes are the normalized intensity and the lateral spread. Solid circles are experimental data, solid line is the present theory, and dotted line is MS treatment. The results of experiments and theories are normalized to the half width of .

(b) Solid line is 50 keV and dotted line is 60 keV. Both of lines are theoretical results. The parameters adopted are = 0.7; and = 0.05. Vertical and horizontal axes are the normalized intensity and the lateral spread , respectively.

(c) Solid line is 100 keV and dotted line is 120 keV. Both of lines are theoretical results. The parameters adopted are = 0.3; and = 0.05. Vertical and horizontal axes are the normalized intensity and the lateral spread , respectively.

Fig. 5 Collisional system is C on O, = 0.1 () and = 1. Solid line is theoretical carve in (a, b, c, d). Vertical and horizontal axes are the normalized intensity and the lateral spread , respectively.

1. Projectile energy is 1 MeV, and = 0.7.
2. Projectile energy is 1 MeV, and = 0.3.
3. Projectile energy is 10 MeV, and = 0.7.
4. Projectile energy is 10 MeV, and = 0.3.

Fig. 6 Collisional system is C on H, = 0.1 () and = 1. Solid line is theoretical curve in (a, b). Vertical and horizontal axes are the normalized intensity and the lateral spread , respectively.

1. Projectile energy is 10 MeV, and = 0.7.
2. Projectile energy is 10 MeV, and = 0.3.

Fig. 1



Fig.2



Fig.3



Fig.4 (a)



Fig.4 (b)



Fig. 4 (c)



Fig. 5 (a)



Fig. 5 (b)



Fig. 5 (c)



Fig. 5 (d)



Fig. 6 (a)



Fig. 6 (b)

