Salman et al. Iraqi Journal of Science, 2022, Vol. 63, No. 5, pp: 1982-1991
DOI: 10.24996/ijs.2022.63.5.13

ISSN: 0067-2904

Stopping Power of Hetero Nuclear Di-Cluster Ions from Partial-Wave Analysis Based on Semi Classical Phase Shifts

Nadher A.Salman, Khalid A. Ahmed, Baida M. Ahmed
Department of Physics, College of Science, Mustansiriyah University, Baghdad, IRAQ

Received: 22/3/2021 Accepted: 5/7/2021 Published: 30/5/2022

Abstract
The mean energy loss per path length, also known as stopping force, is a key quantity that characterizes the interaction of cluster ions with matter. If the internuclear distance in a cluster approaches the interaction range for events, substantial energy transfer is involved. The aim of this theoretical research is to evaluate the electronic stopping power in free electron gas of hetero nuclear di-cluster (He-H) by using a semi classical partial-wave scattering method based on the induced density approach (IDA) model. For ion electron scattering, the transport cross section is used to calculate the energy loss. This method yields a non-perturbative exemplification of energy loss, bridging the difference among classical and quantal representations. The results show the relation of the three kinds of stopping power in (a.u) (cluster stopping power, self-stopping power and correlated stopping power) of hetero nuclear di-cluster ions (He-H) with velocity at different atomic di-cluster distances $(r_{12})(0\ ,1.5\ ,3.5\ ,4.5)$ for different densities($n=10^{22}$, 10^{23}, 10^{24} cm^{-3}) and different temperatures(T=10, 20, 40 eV). It was found that Bragg's peak of stopping power is directly proportional to density and temperature and inversely with atomic di-cluster distance (r_{12}). In literature, there is no information about stopping of hetero di-cluster ions in plasma, therefore, the first time present results needs more attention. The equations in present work were programmed in fortran-90 for numerical calculations.

Keywords: stopping power, phase shifts, transport cross-section, Bragg's peak

قدرة أيقاف الايونات العنقودية الثنائية الذرة الغير متجانسة من تحليل الموجة الجزئية بناء على التقريب الشبه كلاسيكي للأزاحات الطورية

ناظر علي سلمان*، خالد عبد الوهاب أحمد، بيداء محسن أحمد
قسم الفيزياء، كلية العلوم، الجامعه المستنصريه، بغداد، العراق

الخلاصه
الكمية المركزية التي تميز تفاعل أيونات العنقود مع المادة هي متوسط فقدان الطاقة لكل وحدة طول من المسار أو قدرة الأيقاف . هناك نقل كبير للطاقة أذا كانت المسافة بين الذرات للأيونات العنقودية تتجاوز مدى التفاعل مع الألكترونات . تهدف الدراسة النظرية الحالية حساب قدرة الأيقاف الألكترونية في غاز ألكتروني حر لعنقود ثنائي غير متجانس (He–H). تم تطبيق طريقة أستطارة الموجة الجزئية الشبه الكلاسيكية المبينة على موديل تقريب الكثافة المحتثة (IDA), تم التعبير عن فقدان الطاقة عن طريق أنتقال

*Email: nlhhtf@gmail.com

المقطع العرضي لأستطارة ألكترون أيون . يوفر هذا التقريب لفقدان الطاقة تمثيل غير مضطرب والذي يسد الفجوة مابين الوصف الكلاسيكي والكمي . أظهرت النتائج ثلاث انواع من قدرة التوقف بالوحدات (a.u) وهي (قدرة أيقاف العنقود , قدرة الأيقاف الذاتية وقدرة الأيقاف المترابطة) لأيونات العنقود الثنائي الذرة الغير المتجانس (He–H) مع السرعة عند مسافات ذرية مختلفة لعنقود ثنائي (r_{12}) وعند مختلف الكثافات ودرجات الحرارة . وجدنا أن قمة منحني براك لقدرة التوقف تتناسب طرديا مع الكثافة ودرجة الحرارة وعكسيا مع المسافة بين ذرات العنقود الثنائي (r_{12}) . في المراجع لا توجد معلومات حول قدره ايقاف ايونات العنقود الثنائي الغير متجانس في البلازما ويحتاج الى عمل وأهتمام أكثر. المعادلات الموجودة في هذا العمل تم برمجتها بأستخدام برنامج فورتران (90) لغرض الحسابات العددية .

Introduction

Cluster ions' stopping power in the presence of free electrons is important for a number of fields of knowledge, including basic and applied physics, medicine and materials. It has been the focus of extensive research [1]. In literature, several different measurements of ion stopping power in a homogeneous electron-gas process have been suggested. de Ferriis and Arista [2] have calculated the energy loss of charged particles in non-degenerate plasmas using classical and quantum-mechanical approximations. The research yielded basic expressions for the energy loss in terms of particle velocity and charge, as well as plasma density and temperature. Maynard et al. [3] investigated the stopping power of swift heavy ions in both plasma and cold targets, and they developed a single formula from which normal quantum or classical effects can be obtained as precise limits. Arista and Sigmund[4]created a semi-classical theory of ion stopping in matter, with the goal of covering a broad variety of ion energies and mass numbers. This approach provided a nonperturbative energy loss representation that connects the classical and quantal representations. Arista and Clauser [5] studied the energy loss and transport cross section of ionized atomic or neutral beams in plasmas using a semi-classical partial-wave scattering approach according to the WKB approximation. Grande[6]discovered a method for calculating the electronic stopping power and transport cross section of electron-ion binary collisions. The partial wave expansion was used to derive the formula from the induced density of spherically symmetric potential. Matias et al. [1] investigated the electronic stopping of H^{+}projectiles in solid valence electrons. The self-consistent potential for valence-electrons scattering at the projectile was investigated and compared to measurements using the extended Fidel Sum Rule (FSR). F. MAtias et al. [7] used the generalization of the induced density approach (IDA) model to create a nonlinear model for the stopping power of cluster ions based on partial-wave measurement. Therefore, there are several approaches to explain the stopping power in free electron gas like linear response theory presented by Lindhard [8]. Schemes for first-and second-order perturbation[9].and transport cross-section approach[10].

The absence of a unifying method of stopping theory is a major weakness in the present processed. For low Z_1 and high v, Born approximation is a useful method, however, the scope of its applicability is very limited. In the nonattendance of shell correction and high-order terms, this is particularly true. On the other hand, the classical theory of Bohr is an excellent point of beginning the investigation of stopping heavy ions; However, converting it into a quantitative method involves the inclusion of a remarkable number of corrections. The Bloch correction offers a useful connection between the Bohr and the Bethe method. However, the methods mentioned above must be added as a distinct agency. So, the semi-classical phase shift is an attempt to approach the unified theory. The semi-classical theory of ion stopping power in matter aims at a large variety of ion energies and mass numbers [4]. This method offers a non-perturbative interpretation of the energy loss that bridges the distance between quantum and classical concepts [11]. In electron-ion collisions, the mechanical transport cross-section and stopping power have been measured using the induced density method (IDA)[6][1]. The stopping force generated by means of asymmetrical induced charge density on the projectile is used to measure the stopping power. In this case, the non-central induced charge density $n_{ind}(\vec{r})$ is produced by a central Yukawa potential V(r). In the ion's rest frame, the electron–ion collision partial-wave expansions of the stationary wave function in this procedure $n_{ind}(\vec{r})$ is utilized to determine each of the non-central induced potential $V_{ind}(\vec{r})$ or the induced force, $F_{ind}(\vec{r})$ on the ion placement. As a result, this leads to electronic stopping power [7].

The aim of this paper is to evaluate three kinds of electronic stopping power (cluster stopping power, self-stopping power and correlated stopping power) of hetero nuclear di-cluster ions in plasma by applying a semi classical partial wave scattering method based on the induced density approaches (IDA) model. The stopping power was determined using the retarding force caused by the projectile's induced symmetric charge density.

Theory

Computations of the transport cross-section σ_{tr} typically use partial-wave expansion to account for an ion's central potential for electron scattering. Thus, σ_{tr} can be described by phase shifts δ_l, and orbital angular momentum l, from the following equation [12],

$$\sigma_{tr} = \frac{4\pi}{k^2} \sum_l (l+1) sin^2(\delta_l - \delta_{l+1}) \tag{1}$$

where k represents the wave vector associated with the relative position of the scattered electron velocity $v_r = \hbar k/m_e$ and δ_l is the phase shift caused by the scattering of wave components with angular momentum $l = 0,1,1,3, \ldots$. The scattering potential is at the center of this technique $V(\vec{r})$, from which it is possible to quantify phase shifts. The Yukawa potential is [6],

$$V(\vec{r}) = \frac{Z_1 e^2}{r} e^{-r/a} \tag{2}$$

In the present work, a useful model potential has been found. For a particular ion-electron interaction potential $V(\vec{r})$, phase shift might possibly be measured by solving Schrödinger equation by numerical methods [4],

$$\frac{d^2 u_e}{dr^2} + \left(k^2 - \frac{\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2} V(r)\right) u_\ell(r) = 0 \tag{3}$$

In the case of the radial wave equation $u_\ell(r)$, this has the asymptotic type,
$u_\ell \sim \sin(kr - \ell\pi/2 + \delta_\ell)$ at long distance, while the semi-classical WKB approximation provides a formal expression for phase shifts. The phase shift is calculated for a given spherically potential $V(\vec{r})$ by [5],

$$\delta_l = \int dr \sqrt{q^2 - \frac{(l+1/2)^2}{r^2} - \frac{2m}{\hbar^2} V(r)} - \int dr \sqrt{q^2 - \frac{(l+1/2)^2}{r^2}} \tag{4}$$

Using the first-order approximation, a perturbative solution can be found:

$$\delta_\ell^{pert} = -\frac{m_e}{\hbar^2} \int_{r_0}^{\infty} dr \frac{V(r)}{\sqrt{k^2 - (\ell + 1/2)^2 / r^2}} \tag{5}$$

As a result, the transport cross-section is approximated perturbatively [5]:

$$\delta_l^{pert} = \frac{4\pi}{k^2} \sum_l (l+1) \Delta_l^2 \tag{6}$$

$$\text{with} \quad \Delta_l = \delta_l - \delta_{l+1} \tag{7}$$

To get an analytic approximation for cross section of the stopping power, Eq. (1) is rewritten in the form of:

$$\sigma_{tr} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (l+1) \frac{sin^2(\delta_l - \delta_{l+1}) / cos^2(\delta_l - \delta_{l+1})}{1/cos^2(\delta_l - \delta_{l+1})}, \tag{8}$$

$$= \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (l+1) \frac{tan^2(\delta_l - \delta_{l+1})}{sec^2(\delta_l - \delta_{l+1})},$$

$$= \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (l+1) \frac{tan^2(\delta_l - \delta_{l+1})}{1 + tan^2(\delta_l - \delta_{l+1})},$$

$$= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(l+1)\frac{\Delta_l^2}{1+\Delta_l^2} \quad (9)$$

where $\Delta_l = \delta_l - \delta_{l+1}$, with $\tan(x) \approx x$, when $x \ll 1$,

In the limit $\delta_l \ll 1$ and hence $\Delta_l \ll 1$, Eq. (9) is reduced to:

$$\delta_l^{pert} \approx \frac{4\pi}{k^2}(l+1)\Delta_l^2 \quad (10)$$

For massive phase shifts, the perturbation approach is bound to break down. Using Yukawa potential, the phase shifts are reduced to the following equation [2]:

$$\delta_l^{pert} = \eta k_0(x_l) \quad (11)$$

$$\text{with,} \qquad x_l = \frac{l+1}{ka} \quad (12)$$

For large ℓ,

$$\Delta_l = \eta[k_0(x_l) - k_0(x_{l+1})] = \frac{\eta}{ka}k_1(x_l) \quad (13)$$

where $a = \frac{v}{w}$ Bohr's adiabatic radius.

The perturbation approximation does not describe phase shift well for small ℓ. To repair this error, Eq. (13) is multiplied by $\left(l+\frac{1}{2}\right)/(l+1)$ to get [13]:

$$\Delta_\ell = \frac{\left(l+\frac{1}{2}\right)\eta}{\left(l+\frac{1}{2}\right)ka}k_1(x_l) = \left[\frac{\eta}{l+1}\right]x_l k_1(x_l) \quad (14)$$

hence for $x_l \to 0$, $x_l k_1(x_l) \to 1$,

$$\Delta_l = \left[\frac{\eta}{l+1}\right] \quad (15)$$

and hence Eq. (9) becomes:

$$\sigma_{tr} = \frac{4\pi}{k^2}\eta^2\sum_{l=0}^{\infty}\frac{(l+1)}{(l+1)^2+\eta^2} \quad (16)$$

This is an exact result for coulomb scattering. Using Eq. (16), Eq. (9) becomes:

$$\sigma_{tr} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}\frac{(l+1)[\eta x_l k_1(x_l)]^2}{(l+1)^2+[\eta x_l k_1(x_l)]^2} \quad (17)$$

In an electron gas system, the transport cross section was used to calculate the majority of non-perturbative stopping power equations derived from Eq. (1) and the integration of all states within the Fermi sphere. Then the stopping force dE/dz attached to the transport cross section [14] is:

$$\frac{dE}{dz} = \frac{1}{16\pi^2\upsilon^2}\int_{\upsilon-\upsilon_f}^{\upsilon+\upsilon_f} dk\,k^2\,\sigma_{tr}(k)\left[k^2-(\upsilon-\upsilon_f)^2\right]\left[(\upsilon+\upsilon_f)^2-k^2\right] \quad (18)$$

For di-cluster ions, Eq. (18) becomes:

$$\frac{dE}{dz} = \frac{1}{16\pi^2\upsilon^2}\int_{\upsilon-\upsilon_f}^{\upsilon+\upsilon_f} dk\,k^2\,\sigma_{tr}(k)\left[k^2-(\upsilon-\upsilon_f)^2\right]\left[(\upsilon+\upsilon_f)^2-k^2\right][\left(Z_1^2+Z_2^2\right)+2Z_1Z_2\cos(kr_{12})] \quad (19)$$

Results

The equations, in the present work, were programmed using fortran-90 and writing a program (He-H-Dicluster-phasefor) for numerical calculations. Figure 1 shows the variation of stopping power (in a.u.) of He-H di-cluster ions, calculated from Eq. (19), with ion velocity (υ), density(n)=10^{22}cm^{-3} and at temperature(T)=10eV at different atomic di cluster distances r_{12}(in a.u.) ($r_{12} = 0.0 - 4.5$).The results showed that Bragg's peak of cluster stopping power (S_{clstr}) is inversely proportional to the atomic di-cluster distance (r_{12}); this is because the correlated stopping power $S_{cor.}$ depends on r_{12}. The relation between velocity of the di-cluster and stopping power of plasma for different temperatures (10, 20 and 40)eV are shown in Figures (1,2 and 3), respectively. Bragg's peak of cluster stopping power S_{clustr} at $T = 40eV$ is larger than $S_{cluster}$ at $T = 20eV$ and at $T = 10eV$ i.e

$((S_{clustr})_{T=40eV} > (S_{clustr})_{T=20eV} > (S_{clustr})_{T=10eV})$ also S_{clustr} is inversely proportional with r_{12}. Figures (1,4 and 5) represent the stopping power of HeH di-cluster ions with density plasma $(n=(10^{22},10^{23},10^{24})\ cm^{-3})$,respectively at temperature $T=10eV$. Bragg peak of cluster stopping power, S_{clustr} between velocity range $\upsilon_0 < \upsilon \le \upsilon_0 Z_1^{2/3}$ and move toward lower velocity and gets sharper when electron density decreases. While, at high velocity region $\upsilon > \upsilon_0 Z_1^{2/3}$, S_{clustr} decreases faster with increasing velocity and electron density(from $n=10^{22}\,cm^{-3}$ to $n=10^{24}\,cm^{-3}$),as shown in Figures. (1,4,and 5).

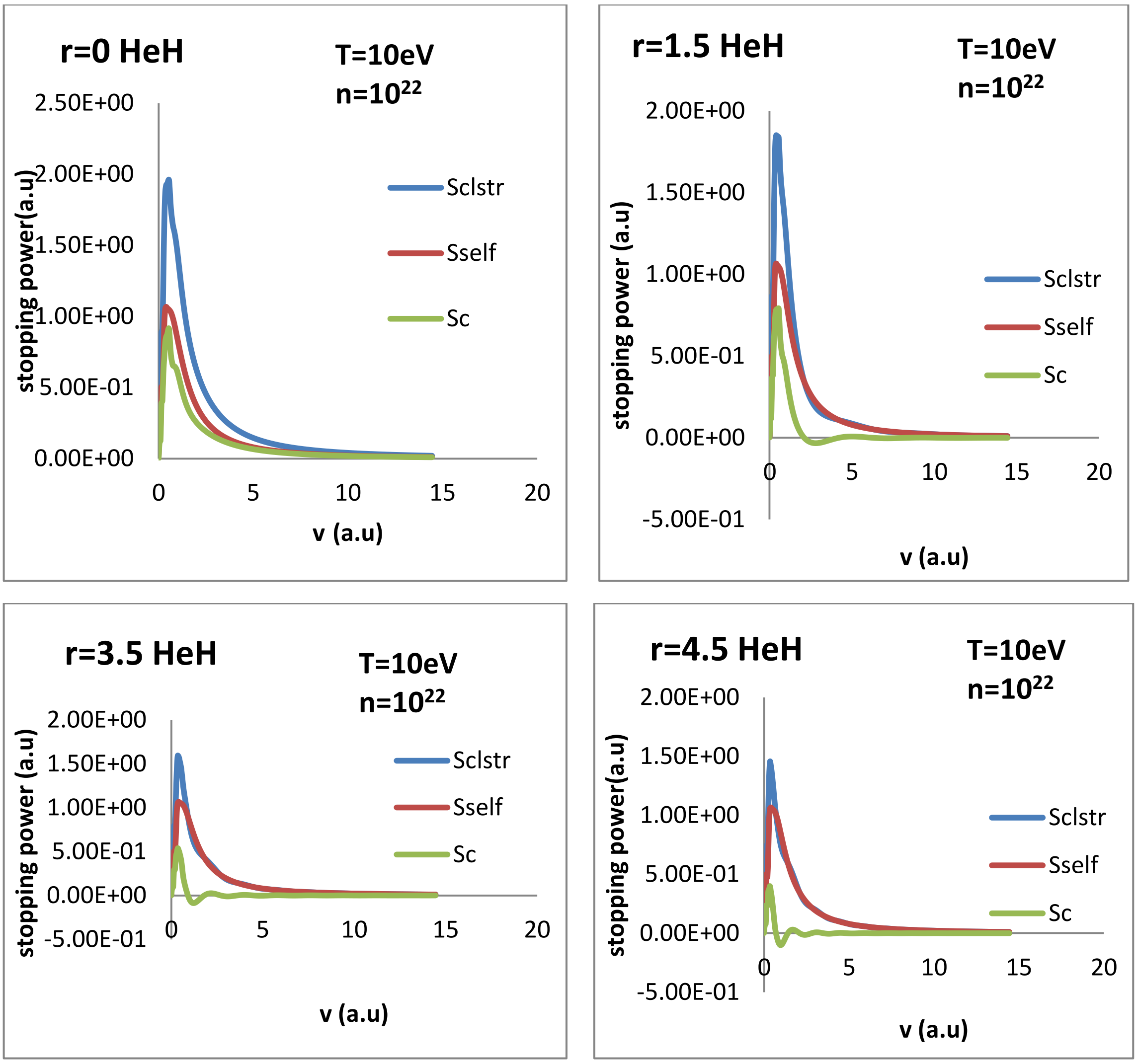

Figure 1-The relation between velocity of the di-cluster and stopping power of plasma using induced density approximation (IDA) (phase shifts problem) with temperature $T = 10ev$ and density $n = 10^{22}cm^{-3}$ for different atomic di-cluster ions distances r_{12} (0 ,1.5 ,3.5 , 4.5).

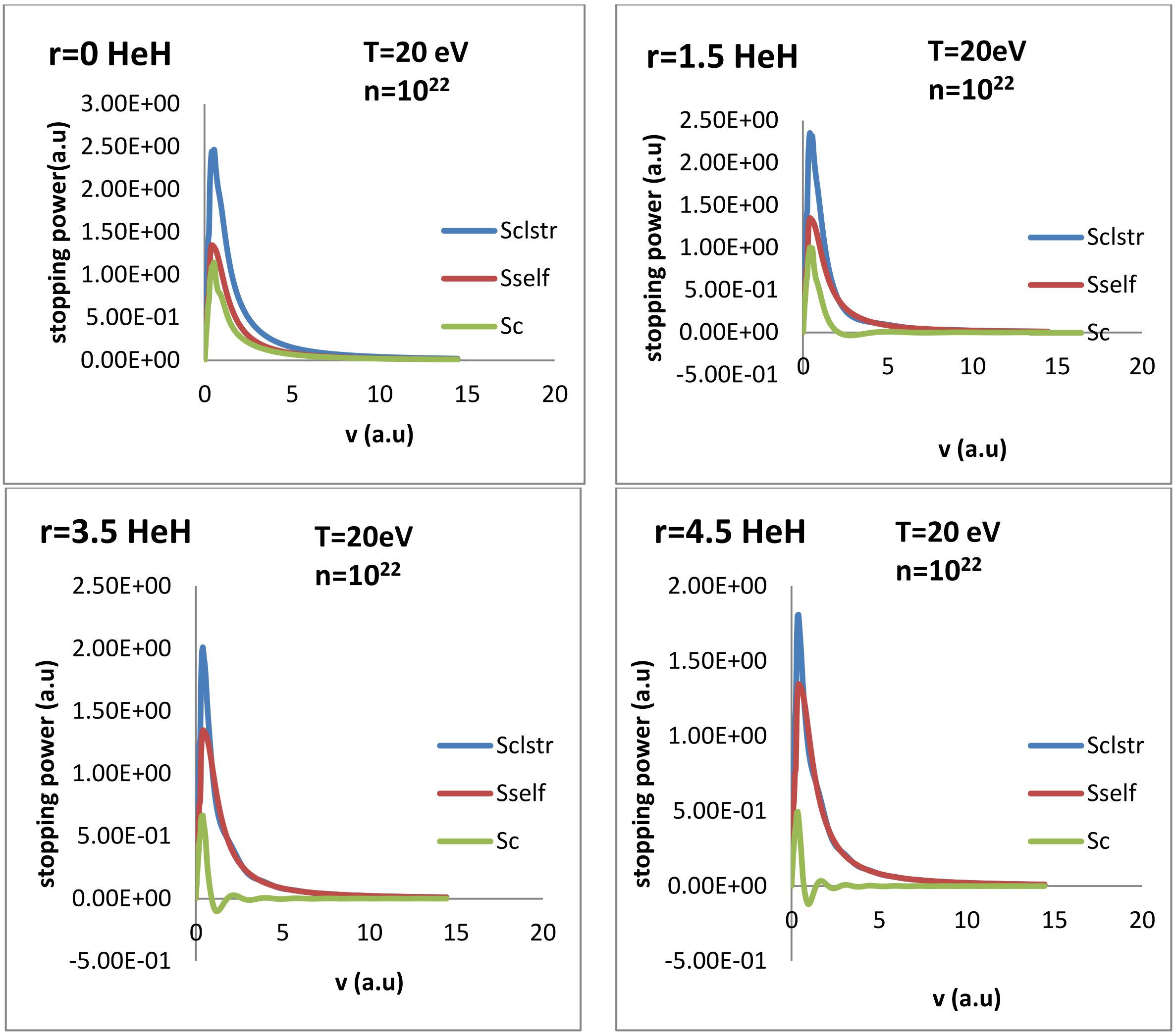

Figure 2-The relation between velocity of the di-cluster and stopping power of plasma using induced density approximation (IDA) (phase shifts problem) with temperature $T = 20ev$ and density $n = 10^{22}cm^{-3}$ for different atomic di-cluster ions distances r_{12} (0 ,1.5 ,3.5 ,4.5)

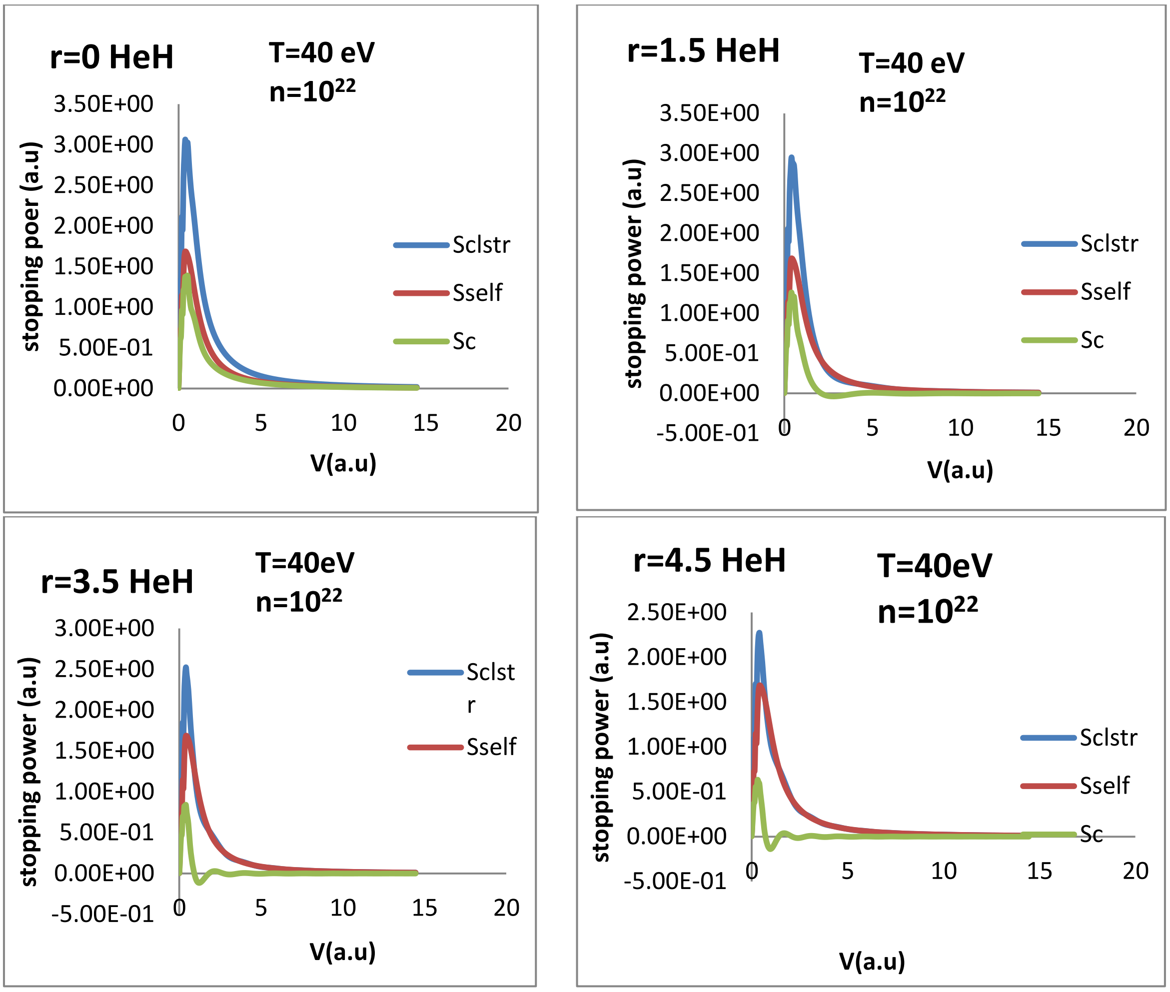

Figure 3- The relation between velocity of the di-cluster and stopping power of plasma using induced density approximation (IDA) (phase shifts problem) with temperature $T = 40ev$ and density $n = 10^{22} cm^{-3}$ for different atomic di-cluster ions distances r_{12} (0 ,1.5 , 3.5 , 4.5)

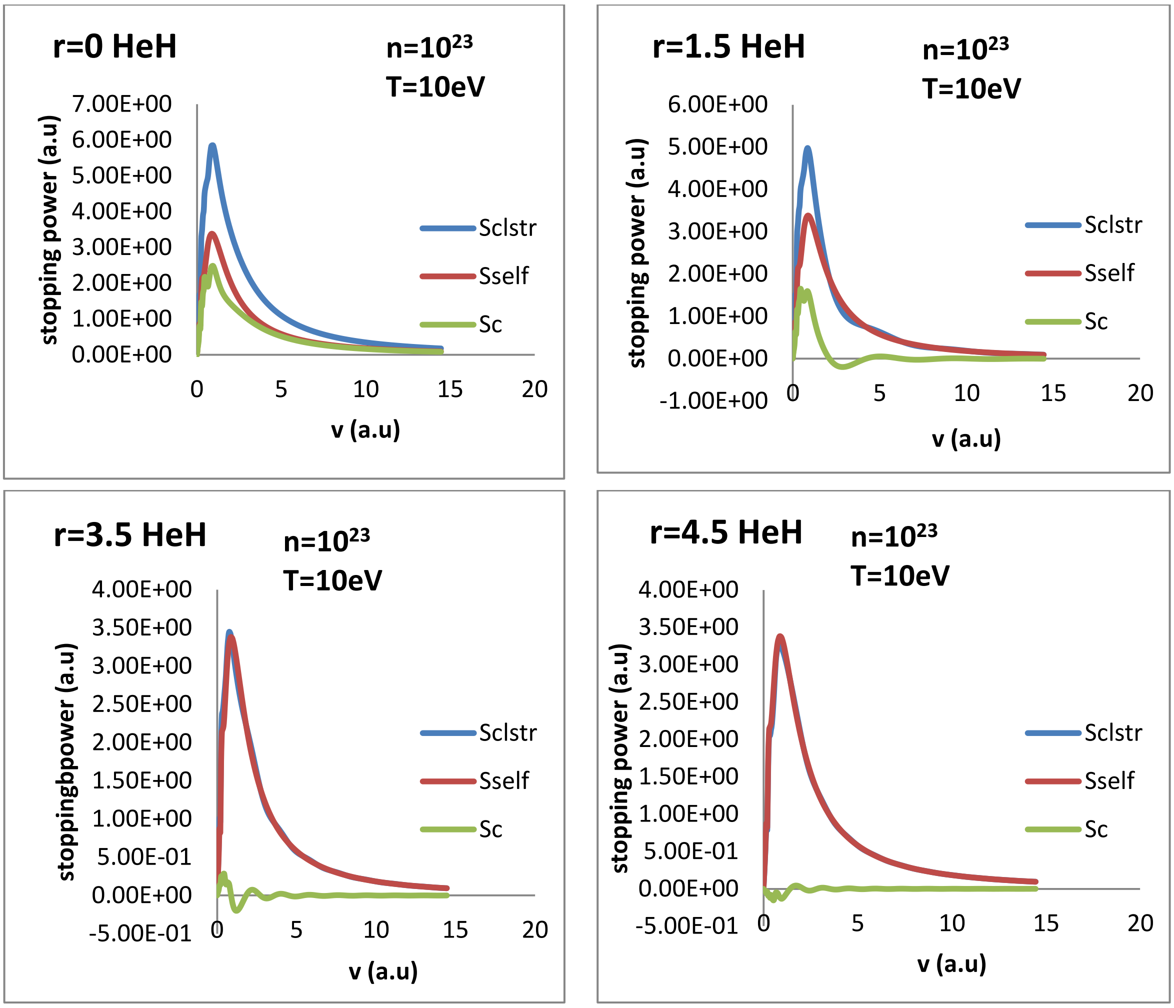

Figure 4-The relation between velocity of the di-cluster and stopping power of plasma using induced density approximation (IDA) (phase shifts problem) with temperature $T = 10ev$ and density $n = 10^{23} cm^{-3}$ for different atomic di-cluster ions distances r_{12} (0 ,1.5 , 3.5 , 4.5)

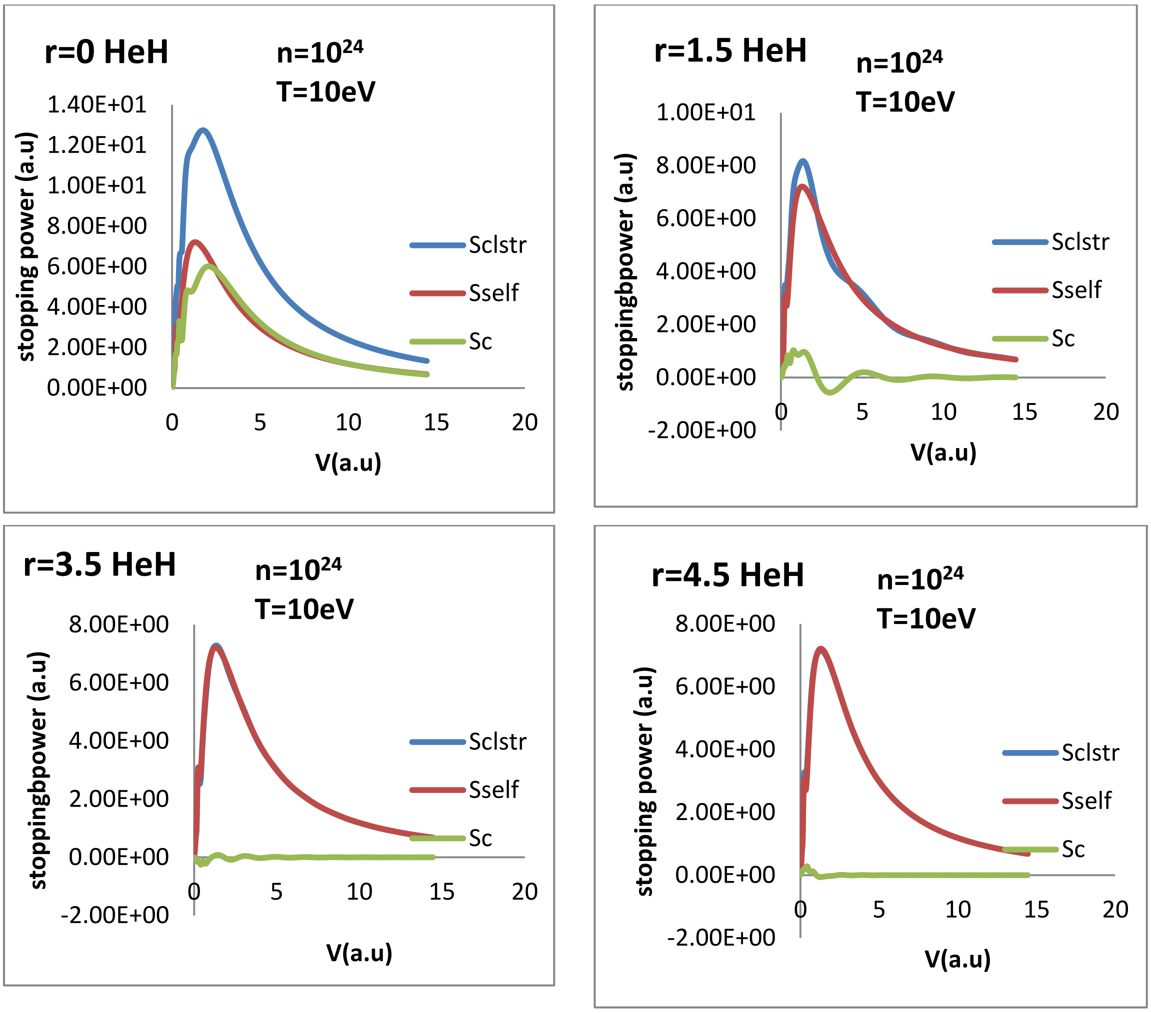

Figure 5- The relation between velocity of the di-cluster and stopping power of plasma using induced density approximation (IDA) (phase shifts problem) with temperature $T = 10ev$ and density $n = 10^{24} cm^{-3}$ for different atomic di-cluster ions distances r_{12} (0 ,1.5 , 3.5 , 4.5)

Conclusions

The energy loss of hetero nuclear di-cluster (He-H) in plasma calculated in the current work was centered on the effects of a partial wave study. It was built via the popularization of the Induced Density Approach (IDA) pattern. Stopping power based on semi-classical phase shift is strongly dependent on transport cross-section σ_{tr} where σ_{tr} depends on the relative velocity $v_r = |v - v_e| = \frac{\hbar k}{m}$ and phase shift δ_ℓ It was found that Bragg's peak of stopping power was directly proportional to density and temperature, but not on the center of the peak. Increasing the density and temperature lead to the increase in the collisions between hetero nuclear di-cluster and electronic targets that help to stop the hetero nuclear di-cluster in the medium such as plasma.

References

[1] F. Matias *et al.*, "Ground-and excited-state scattering potentials for the stopping of protons in an electron gas," *J. Phys. B At. Mol. Opt. Phys.*, vol. 50, no. 18, p. 185201, 2017.

[2] L. de Ferrariis and N. R. Arista, "Classical and quantum-mechanical treatments of the energy loss of charged particles in dilute plasmas," *Phys. Rev. A*, vol. 29, no. 4, p. 2145, 1984.

[3] G. Maynard, G. Zwicknagel, C. Deutsch, and K. Katsonis, "Diffusion-transport cross section and

stopping power of swift heavy ions," *Phys. Rev. A*, vol. 63, no. 5, p. 52903, 2001.
[4] N. R. Arista and P. Sigmund, "Stopping of ions based on semiclassical phase shifts," *Phys. Rev. A*, vol. 76, no. 6, p. 62902, 2007.
[5] C. F. Clauser and N. R. Arista, "Energy loss and Z oscillations of atomic beams in plasmas," *Phys. Rev. E*, vol. 88, no. 5, p. 53102, 2013.
[6] P. L. Grande, "Alternative treatment for the energy-transfer and transport cross section in dressed electron-ion binary collisions," *Phys. Rev. A*, vol. 94, no. 4, p. 42704, 2016.
[7] F. Matias, R. C. Fadanelli, P. L. Grande, N. R. Arista, N. E. Koval, and G. Schiwietz, "Stopping power of cluster ions in a free-electron gas from partial-wave analysis," *Phys. Rev. A*, vol. 98, no. 6, p. 62716, 2018.
[8] J. Lindhard, A. Winther, and others, *Stopping power of electron gas and equipartition rule*. Munksgaard, 1964.
[9] J. M. Pitarke, R. H. Ritchie, and P. M. Echenique, "Quadratic response theory of the energy loss of charged particles in an electron gas," *Phys. Rev. B*, vol. 52, no. 19, p. 13883, 1995.
[10] N. R. Arista, "Energy loss of ions in solids: Non-linear calculations for slow and swift ions," *Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms*, vol. 195, no. 1–2, pp. 91–105, 2002.
[11] N. F. Mott and H. S. W. Massey, "*The theory of atomic collisions, chap." Oxford University Press, London, England*, 1949.
[12] C. F. Clauser and N. R. Arista, "Stopping power of dense plasmas: The collisional method and limitations of the dielectric formalism," *Phys. Rev. E*, vol. 97, no. 2, p. 23202, 2018.
[13] L. D. Landau and E. M. Lifshitz, *Quantum mechanics: non-relativistic theory*, vol. 3. Elsevier, 2013.
[14] L. D. Landau and E. M. Lifshitz, "*Statistical Physics, Part 1: Volume 5*," 1980.