

SRI VENKATESWARA INTERNSHIP PROGRAM FOR RESEARCH IN ACADEMICS (SRI-VIPRA)





## Project Report of 2024: SVP-2417

"Ion Coulomb Explosion of spherical clusters with varying

<u>charge Density</u>  $\rho = \rho_{\circ} \left(1 - \frac{r^3}{r_o^3}\right)^2$ 



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#### **SRIVIPRA PROJECT 2024**

Title : "Ion Coulomb Explosion of spherical clusters with varying charge Density

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### **Certificate of Originality**

This is to certify that the aforementioned students from Sri Venkateswara College have participated in the summer project SVP-2417 titled "*Ion Coulomb Explosion of spherical clusters with varying charge Density*  $\rho = \rho_{\circ} \left(1 - \frac{r^3}{r_{\circ}^3}\right)$ ". The participants have carried out the research project work under my guidance and supervision from 1<sup>st</sup> July, 2024 to 30<sup>th</sup> September 2024. The work carried out is original and carried out in an online/offline/hybrid mode.

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I am really thankful to all who were directly or indirectly involved with me over this project.

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## **ABSTRACT**

A collision less model of Ion Coulomb explosion of clusters in a volume of gas is studied. A short Gaussian laser pulse immediately turns the cluster into a plasma ball via tunnel ionization. After the complete evacuation of the electrons, the ion coulomb explosion of the cluster takes place. The electric field and potential is dependent upon the density variation of the cluster since the charges implicitly give rise to the repulsions. The ion energy distribution function due to a single cluster is first calculated and then the same is considered for all the clusters in the laser channel that ionize. The electric field so created is dependent on the radius of the cluster and as the Ion coulomb explosion takes place, the ions start moving away from the centre and the electric field decreases.

A laser with intensity just suitable to remove electrons from the cluster lets the ions gain enough energy to collide with each other and the atoms or molecules from the surrounding gas, to undergo fusion reaction and produce neutrons with suitably high yields. The so obtained ions and neutrons can be further harnessed to study their energies and use laboratory experiments, if required.

Variations in the cluster densities is studied including-

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ho}=oldsymbol{
ho}_{\circ}\left(1-rac{r^3}{r_{\circ}{}^3}
ight)$$

The density variations give peculiar results of the ion energy distribution functions and the number of neutrons of the order of ~ $10^5$  neutrons/ Joule. The ions so produced can generate neutrons with reasonably high yields. The scheme may also find application in tokamak fusion. The energy plots so obtained vary with the initial radius of the ion under consideration. They are continuous plots rising to a peak and falling thereafter. The ion energy distribution function plots also show dependence on the initial radius of the ion and is a continuous plot with sudden increase in the slope near the maximum value of the energy gain.

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# Chapter 1

## **INTRODUCTION**

### 1.1 Plasma: A fourth state of matter

Plasma state is identified as the fourth state of matter for the fact it shows various peculiar properties different from the three known states namely solid, liquid and gas. It may be formed from one or more electrons being stripped away from the neutral molecules leading to formation of positively charged ions and free electrons coexisting in the same region of space. The volume containing the plasma may be as a whole neutral but charge on individual particle isn't zero. For this fact, the electric and magnetic fields interact very differently with the plasma state as compared to the other three states of matter. In addition to responding to the external fields, the plasma state also shows some collective coherent properties over large ranges because of the internal electric and magnetic fields self created owing to the presence of concentrated charges in one region as compared to the other regions and also the differential movements of ions and electrons which produces current.



Figure 1:Plasma and other state of matter of matter as increasing energy Source:Google<sup>[27]</sup>

Plasmas are generated by supplying energy to a neutral gas causing the formation of charge carriers<sup>[1-3]</sup>.When sufficient amount of energy is provided to a gaseous volume Figure 1: Plasma and other states of matter as increasing energy Source:Google<sup>[27]</sup> for the electrons to leave the atoms un-neutralized and form coexisting oppositely charged particles in the same space. The energy supplied can be in the form of heat, mechanical stress as well as electromagnetic energy.Various ways of providing energy include heating, by adiabatic compression or over flame directly, to sufficient temperatures, via energetic beams that transfer energy to the gases through collisions, by applying electric field to the gases through which few free electrons get accelerated and over collision with neutral atoms release electrons.

**NON LINEARITY IN PLASMA**. Plasma shows non-linear interaction with light. The higher order terms for the expression of the effective polarization become extremely important and can't be ignored when the electric field of a large magnitude interacts with the plasma.

 $P = \in 0 [E^{\rightarrow} \chi 1 + E^{\rightarrow} E^{\rightarrow} \chi 2 + E^{\rightarrow} E^{\rightarrow} \chi 3 + \ldots + E^{\rightarrow} n \chi n]$ 

We now consider higher order terms with  $\vec{E}$  in the expression and this gives rise to various non-linear effects on the interaction of  $\vec{E}$  with high amplitudes. One parameter that characterizes the strength of the nonlinear interaction between the incident laser and the plasma is the oscillating velocity,  $v_0$ , of the electron in the electromagnetic field<sup>[23]</sup>. This parameter can be expressed in terms of laser intensity  $\frac{v_o}{c}$  = 8.55 \* 10<sup>-10</sup> $\lambda_{\mu}I$ . When the electrons in a plasma are and wavelength as, subjected to such a huge force, several effects such as harmonic generation, simulated Brillouin and Raman scattering, degenerate and resonant four wave mixing, self-focusing and parametric amplification are set in the plasma. These phenomena are characterized by the generation of one or more scattered e.m. waves that may have a different frequency and direction than the incident e.m. wave <sup>[23]</sup>. In addition, plasmas demonstrate certain unique nonlinear phenomena such as nonlinear mode conversion, parametric decay instability, two plasmon decay and relativistic self-focusing <sup>[23]</sup>. These effects occur simultaneously in plasma giving it its unique properties of interaction with the EM-waves. One of the nonlinear processes discovered soon after the laser was born is self-focusing. This occurs because the refractive index of a medium gets modified by the light and a focusing nonlinear lens can be formed by the Gaussian transverse spatial profile of the propagating laser beam <sup>[9]</sup> inside the amplifiers, leading to such large intensity that the amplifying medium or other optical components break down.

### **1.2 Coulomb Explosion: an Overview**

The propagation of intense short pulse laser through under-dense plasma is known to produce completely electron evacuated ion channel in the axial region of the laser<sup>[4-9]</sup>. The laser exerts radial ponderomotive force on electrons and pushes them out on the time scale of a plasma period<sup>[10]</sup>.

The ponderomotive forces represent time-averaged nonlinear electromagnetic forces acting on the plasma in the presence of oscillating electromagnetic fields<sup>[22]</sup>. The charged particles experience unbalanced electromagnetic force in the two half cycles and therefore they are forced to move towards the regions of lesser field strength. The electric and magnetic forces of the laser are perpendicular and therefore, the simultaneous action of the two forces act on the particles. The ponderomotive forces are usually divided into various categories, in particular, distinguished by their dependence on temporal or spatial wave intensity derivatives<sup>[22]</sup>.



Figure 2: Ion Coulomb Explosion of a cluster Source: Google<sup>[28]</sup>

This process is known for efficient transfer of energy from the lasers to ions. Various studies have been done on how the process of this energy transfer takes place and how the internal mechanism works. Coulomb explosion turns out to be the best suited Figure 2 : Ion Coulomb Explosion of a cluster Source: Google<sup>[28]</sup> potential mechanism for the same. When the gas contains clusters of molecules, the clusters ionize forming spherical balls consisting un-neutralized positive charges leading to high repulsions due to electrostatic force thereby resulting in the ion coulomb explosion of these spheres of ions. The inter ionic repulsions due to electrostatic force that arise owing to un-neutralized charges on the excursion of electrons overcome the hydrodynamic pressure of the sphere and the ions gain energy and start to move apart from one another. The energy gained by these ions depends upon

the excursion of electrons caused by the laser field. Further, when these ions collide with each other, interactions such as fusion reactions take place and neutrons are released. Often, the interactions also produce high energy waves in the form of X-rays. The predicted results by this process for various experiments have also been verified.

### 1.3 Interaction of laser pulses with plasma

In recent years, much effort has gone into the understanding of the interaction of short  $(10^{15}W/cm^2)$  laser pulses with matter <sup>[11]</sup>. These experiments have typically involved studying the interaction of these high intensity laser pulses with either a low-density gas (<  $10^{19}atoms/cm^3$ ) or a high-density solid target (>  $10^{23}atoms/cm^3$ ). Many of these studies have been motivated by a desire to generate photons and particles with energies far above the energy of a single laser photon. In particular, some of these experiments have investigated the production of incoherent and coherent x-ray radiation or the generation of energetic electrons <sup>[12]</sup>. The intensity of the laser is high enough to sufficiently rattle the electrons and produce non-linear effects in the medium. The high amplitude and intensity of the laser pulse produces several oscillating modes for the electrons with sufficiently high energy thereby showing unique effects.

A high intensity (>  $10^{16}W/cm^2$ ), ultrashort (100 fs) laser pulse explosively ionizes a solid and creates a high-density plasma with temperatures of the order of millions (10<sup>7</sup>) of Kelvin, 10<sup>9</sup> bar pressures,  $10^{12}$  A/cm<sup>2</sup> electron currents, and giant (10<sup>8</sup> Gauss) 'quasi-DC' magnetic fields – in short, intra-stellar conditions. The giant magnetic fields, the largest available terrestrially, have been known to play a crucial role in the transport of electrons in these plasmas and are of immense interest for potential applications in hybrid (inertial and magnetic) confinement in laser fusion, and for the recently proposed fast ignition laser fusion scheme. Since the first observation of such a magnetic field, their origin, magnitudes and other qualitative features have attracted considerable attention. This technique uses the change of polarization state of a weak 'probe' beam caused by the huge magnetic field generated when a strong 'pump' laser beam hits a solid surface. The main result is the first demonstration of ultrashort, megagauss magnetic pulses, with pulse duration in the picosecond range and having a peak value of ~30 MG <sup>[24]</sup>.

Ditmire et al. <sup>[11]</sup> have observed 95% laser energy absorption in a deuterium gas jet target with deuterium (D) clusters of 60 Å size, producing 2.5 keV ions at a laser intensity of  $Il = 2 * 10^{16}W/cm^2$  at 0.82 µm wavelength. These ions produce neutrons via D–D reaction with an efficiency of 10<sup>5</sup> neutrons/J of incident laser energy <sup>[13]</sup>. The presence of clusters enhances the absorption of energy because energy is transferred from the laser to the ions as well. When there are no clusters, only the molecules present in the laser channel interact with the pulse and since in an under dense plasma column, the number is quite less, thus energy transfer is limited. When there are no clusters in the gas jet, the absorption of laser energy is only 5% and no neutrons are observed. A similar study by Ditmire with Xe clusters reports  $Xe^{40+}$  ions with kinetic energy up to 1 MeV at  $I_l = 2 * 10^{16}W/cm^2$ . Recently Madison et al have observed Coulomb explosion at relativistic intensities <sup>[13]</sup>.

### **1.4 Prior studies on the Coulomb Explosion**

Ditmire et al. <sup>[12]</sup> developed a model to explain those experimental findings of ion coulomb explosion of clusters. The laser ionizes the clusters through tunnel ionization and turns the gas into collisional plasma. The electrons that are released collide with other molecules and cause their ionization as well. The energy gained by the electrons due to the electric field of the laser is enough for them to leave the spheres positively charged and the ions thus undergo ion coulomb explosion due to the Coulomb repulsion dominance over the hydrodynamic pressure of the sphere. But the collisional model of electron heating appears questionable for low atomic number clusters, even when their cluster radii are greater than 50 Å, as electron mean free path at electron density  $ne = 10^{22}/cm^3$ , electron kinetic energy nearly 2 keV in a deuterium plasma is around 10000 Å, which is much bigger than the cluster size <sup>[13]</sup>. There are a very few chances of an electron colliding with the other ions and therefore another collisionless models of the explosion have been developed.

Milchburg et al <sup>[14]</sup> have developed a one dimensional hydrodynamical code to study laser interaction with time-dependent plasma hydrodynamics of the heated cluster. They found that the electron density profile is non-uniform and the resonance at the critical layer plays a significant role in the laser coupling <sup>[13]</sup>. Zweiback et al. <sup>[15]</sup> have developed a theoretical model of collisionless ion Coulomb explosion from clusters fully depleted of electrons. This model gives ion energy distribution function from a single cluster as(*E*)  $\propto E 1/2$ , up to a cutoff energy and zero beyond it <sup>[13]</sup>. C. S. Liu and

*V.K.Tripathi*<sup>[13]</sup> have modeled the ion coulomb explosion of clusters when a laser with Gaussian radial distribution of intensity irradiates the gas and forms plasma through tunnel ionization of the clusters. In this case, the oscillatory electron velocity due to the laser field is comparable to the potential energy of the electron due to the cluster therefore partial evacuation of the electrons is considered. Therefore a certain region of the sphere remains un-neutralized and the expression for the energy gain by the ions and their energy distribution function for the specified case are obtained.

### 1.5 Current Modeling

The densities of the clusters in the above modeling are considered to be constant. We have tried to model the ion coulomb explosion of the clusters with varying charge densities. As the radius of the cluster increases, the charge density varies depending upon r.

The form of the density that we have considered is:

$$\rho = \rho_o \left(1 - \frac{r^3}{r_o^3}\right)$$

The complete evacuation of electrons with excursion more than twice the radius of the cluster is considered. The partial evacuation brings in the effect of magnetic field and thus the motion of the electrons becomes complicated with the velocity becoming inharmonic and the motion also doesn't remain simple harmonic.

A Gaussian laser pulse of duration in femtoseconds causes tunnel ionization of the clusters of deuterium-tritium gas channel forming plasma balls of positive charge. The inter-ionic repulsion force pushes the ions away from one another. As the ions move apart, they accelerate and gain energy in the electrostatic field. The ions then collide with each other and other ions and molecules in the channel. The deuterium-tritium ions and molecules collide releasing a good number of neutrons after the fusion reaction. Since it is not mandatory for all the moving ions to collide, the collisional cross-section of the deuterium ions at 2.5 keV electron energy is considered to calculate the number of neutrons for both the densities.

The graph of energy gain of the ions with the radius  $r^3/r_0^3$  is plotted and the graph of ion energy distribution function is plotted with respect to the energy gain. The plots of energy with the initial radius show a peak and then fall monotonously. The plots for the ion energy distribution function with the energy gives a positive slope with the gradient of slope increasing slowly at first and then a very sharp increase near the maximum energy gain by the ions.

Comparative analysis for the energy with radius plots for both the densities show that they behave in a similar manner for small region of the plot when the initial radius of the ions is close to 0, i.e. for the ions near the centre of the cluster. Also, the ion energy distribution with initial energy gain plot is similar except for the number of the neutrons produced. Both the densities show same variations. The comparative analysis is beneficial to know the effect of the density variation on the energy gain and ion energy distribution. This also helps to predict the number of neutrons produced in each case.

### 1.6 Some applications of Coulomb Explosion

Coulomb explosion finds applications in different fields including,

(i)Coulomb explosion imaging, where a fast tri-atomic molecular ion impinges on a thin foil that strip off the electrons, leading to the repulsion of the positively charged remnants and freezing of the velocities up to an imaging detector where the initial molecular structure may be traced back.

(ii) Source of soft and hard x -rays , the x -ray yield may be cluster size and density of clusters dependent.

(iii) Source of pulsed and fast neutrons generated in appropriate gas jets, like those containing deuterium (D) or tritium (T). The neutrons are the result of D-D or D-T interactions of fast elements ejected from different clusters. The neutron yield depends on cluster size and laser parameters.

(iv)Simply a way for achieving fusion, since exploding clusters provide sufficient kinetic energy for deuterons to trigger a fusion reaction. An alternative would be the use of the energetic ions for heating a pre-compressed D-T pellet up to ignition <sup>[17-20]</sup>

# <u>Chapter 2</u>

# **IMPORTANT CONCEPTS**

### **2.1 COULOMB's FORCE AND ITS LIMIT**

By virtue of charges on the particles, they attract and repel each other. Point like charges repel and point unlike charges attract. As the size of the particles increase, the attraction and repulsion behavior may vary due to induction of charges as the inter-particle distances vary. The electrostatic force or the Coulomb's force vary as the inverse of square of the inter-particular distance.

As the inter particle distance reduces to the units of radius of the nucleus, the nature of the particles become unimportant and the nuclear forces dominate which are purely attractive in nature. This is the limit of Coulomb's law where it seizes to act and the nuclear forces come into picture.

$$F = \frac{k.q1q2}{r^2}$$

'k' being a constant.

The force is considered to act upon the stationary charges. As the charges accelerate, the combined effect of electromagnetism comes into picture and the force is modified to Lorentz force, also including the force due to the induced magnetic field as well as applied, if any.



Figure 3: Electrostatic interaction between Nucleus and surrounding electrons Source: Google<sup>[29]</sup>

# 2.2 ELECTROSTATIC POTENTIAL AND THE ACCELERATION OF IONS

Due to the presence of unbalanced charges in a region, an electrostatic potential develops and the charges brought in the region of the existing potential, experience force in the direction from higher to lower potential regions. The Coulomb's force is the negative gradient of the electrostatic potential. It is defined as the amount of work done in bringing a unit positive charge from a reference point to a specific point in a region of the field without any acceleration.

$$V = \frac{kQ}{r}$$

As the ions in a cluster are like charged particles with inter particle distances being very small yet greater than the Coulomb's limit, the force is enough to accelerate the ions away from each other due to the electrostatic potential difference.

### 2.3 WORK DONE AND ENERGY GAIN BY THE IONS

The work is done by the field on the charges to accelerate them. As the charges in the region of an electric field accelerate, they gain energy. The transformation of energy from the field's stored energy to the kinetic energy of the charges takes place. From the equation,

$$\frac{1}{2}mv^2 = \int_a^b \overrightarrow{E}. \, \overrightarrow{dr} \qquad (eq. 2.1)$$

the kinetic energy is stored in the charges by virtue of their motion and as the charges further collide with each other or the surrounding boundaries, various changes in their motion arise depending upon the initial energy before interaction.

### 2.4 GAUSS's LAW

Gauss's Law of electrostatics relates the net electric flux passing through a closed region to the charge enclosed in the region, where Electric flux is defined as the Electric field multiplied by the normal component of the area vector.

Mathematically,

$$\epsilon \oint \vec{E} \cdot \vec{dr} = charge \ enclosed \ in \ the \ region \qquad (eq. 2.2)$$

where, the integral is over the closed surface, epsilon is the permittivity of the region and charge enclosed is the net sum of all the discrete as well as continuous charge distributions within the region under consideration.



### 2.5 ELECTROMAGNETIC WAVES AND THE ENERGY STORED

Electromagnetic waves are transverse waves with electric and magnetic fields oscillating in perpendicular directions and mutually perpendicular to the direction of propagation as well. These waves do not require any material medium to travel and can propagate through vacuum as well because the energy propagates as the fields and they do not require any external medium particles to oscillate and transfer energy.

The electromagnetic spectrum can be divided into various sections depending upon the frequency and thus the energy of the waves including radio-waves ( $f < 10^9$ Hz), microwaves ( $10^9 < f < 10^{11}$ Hz), infra-red waves ( $10^{11} < f < 10^{14}$ Hz), visible rays ( $4 * 10^{14} < f < 7.5 * 10^{14}$ Hz), ultraviolet rays ( $7.5 * 10^{14} < f < 10^{16}$ Hz), x-rays ( $10^{16} < f < 10^{19}$ Hz), gamma rays ( $10^{19} < f < 10^{22}$ Hz) and cosmic rays ( $f > 10^{22}$ Hz) in the increasing order of their frequency and energy, microwaves being the leaat and the cosmic rays being the most energetic rays.

#### **Electromagnetic Wave**



Figure 5: Electromagnetic wave: Electric And Magnetic field perpendicular to direction of propagation Source: google<sup>[31]</sup>

The energy is stored in the electromagnetic waves in the form of electric and magnetic fields. The energy density, i.e. energy stored per unit volume is distributed equally in both the forms, magnetic as well as electric, therefore the EMW can do both electric and magnetic work equivalent to the energy stored. The energy stored is proportional to the square of the amplitude to these fields.

For the waves travelling in vacuum,

$$E_{y} = E_{o} \sin (wt - kx)$$
  

$$B_{z} = B_{o} \sin (wt - kx)$$
  

$$u_{e} = \frac{1}{2} \varepsilon_{o} E^{2} \qquad u_{b} = \frac{1}{2\mu_{o}} B^{2}$$
  

$$u = u_{e} + u_{b} = \varepsilon_{0} E^{2} = B^{2} / \mu_{o}$$
(eq.2.3)

The energy density is constant throughout the space and time and this energy can be used to transfer energy in the form of quanta as photons to a target that they strike.

In any medium other than vacuum, the energy modifies by  $\varepsilon 0$  to  $\varepsilon$  and  $\mu 0$  to  $\mu$  where  $\varepsilon$ ,  $\mu$  depend upon the properties of the medium in which the waves travel.

Let P is the energy transported per unit time across a unit cross-sectional area perpendicular to the direction in which the wave is travelling. Consider a plane electromagnetic wave propagating along the x-axis. The wave propagates a distance cdt along the x-axis in a time interval dt. If we consider a cross-sectional area A at right-angles to the x-axis, then in a time dt the wave sweeps through a volume dV of space, where dV = Acdt. Therefore the amount of energy in this volume is

 $dW = wdV = \varepsilon_0 E^2 Acdt$ 

Thus the power per unit area carried by the wave is given by

$$P = \frac{dW}{A \, dt} = \varepsilon_0 E^2 A c \frac{dt}{A \, dt}$$

$$P = \varepsilon_0 c E(cB) = \varepsilon_0 c^2 E B = \frac{EB}{\mu_0}$$

$$P = \frac{EB}{\mu_0}$$
(eq. 2.4)

Thus,

It specifies the power per unit area transported by an electromagnetic wave at any given instant of time. The peak power is given by

$$P_o = E_o B_o / \mu_o$$

It is easily demonstrated that the average power per unit area transported by an electromagnetic wave is half the peak power, so that

$$I = \overline{P} = \frac{E_o B_o}{2 \mu_o} = \frac{\varepsilon_o c E_o^2}{2} = \frac{c B_o^2}{2\mu_o}$$

### **2.6 GAUSSIAN LASER PULSE**

A light beam is, in general made up of various waves of different frequencies which superpose to give the resultant beam. A laser beam is a monochromatic beam of light consisting of a single frequency that is amplified through the laser device that amplifies light by stimulated emission of radiation.

Gaussian beams are the lowest-order self-consistent field distribution in optical resonators provided that there are no intra-cavity elements causing beam distortions. For that reason, the output beams of many lasers are Gaussian. Moreover, the Gaussian distribution remains unaltered over the wave equation in a medium, i.e.

there are changes only in the parameters whereas the form of the beam doesn't change. These beams are usually considered with small beam divergence therefore, the first order approximation can be applied while solving the propagation equation in any medium and the higher order terms thus omitted result in the same type of function with some modified parameters.

A laser pulse of sufficient intensity and duration of femto-seconds, when launched into a gaseous medium possess the capability to ionize the gas and form plasma. When the gas contains clusters of molecules, the clusters ionize forming spherical balls consisting high positive charges and leading to high repulsions thereby resulting in the ion coulomb explosion of these spheres.

One form of a pulsed Gaussian laser beam is represented as  $E_t = \hat{x} A(t, r, z) e^{-i(wt-kz)}$ 

$$\dot{z}_L = \dot{x} A(t, r, z) e^{-t(wt - \kappa z)}$$

$$A_{x=0}^2 = A_o^2 e^{-\left(\frac{R^2}{R_o^2}\right)}$$

where  $R_o$  is the radius of the Gaussian pulse<sup>[13]</sup>



Figure 6:Gaussian laser pulse Source: Google<sup>[31]</sup>

### **2.7 TUNNEL IONIZATION BY A LASER**

Inside an atom or a molecule, the electrons are bound to the nucleus through coulomb force between opposite charges. The electrons lie inside a potential well created around the nucleus and do not have sufficient amount of energy to cross the well and come out of it, therefore it remains bound there. Yet, according to Quantum formulation, the probability of the electron being found out of that well is still not zero as the Heisenberg's Uncertainty principle would then imply that if the certainty in the particle's existence in a certain region is precise, its momentum will be highly uncertain.

As a laser is incident on the molecules, the net electric field experienced by the electrons alters due to the electric field of the laser. The effective potential takes a new form and it reduces the size of the potential barrier that electrons have to cross to be out of the cluster. The probability of the electrons escaping the barrier

increases and the clusters ionize. The accompanying diagram depicts the alteration of the electric field experienced by the electrons which increases the chance of escape.



Figure 7: Tunnel ionization of electrons by laser field Source: Google<sup>[33]</sup>

### **2.8 DENSITY OF STATES**

The number of possible states that can be occupied per unit volume is known as the density of states. For any spherical volume,

$$dN = 4\pi r^2 n_o dr \tag{eq. 2.5}$$

where, dN gives the number of particles present in the small volume  $4\pi r^2 dr$ .

When the above expression is related to the energy depending upon r, the equation transforms to give energy density of states.

$$dN = (E) \tag{eq. 2.6}$$

here, f(E) gives the density of states.

The expression can be transformed as  $dN = 4\pi r^2 \frac{dr}{dE} dE$ 

Thus,

$$f(E) = 4\pi r^2 \frac{dr}{dE} dE \qquad (eq. 2.7)$$

The relation between dr and dE can be derived according to their dependence on each other.

### **2.9 COLLIOSIONAL CROSS-SECTION AREA**

When two charged particles approach each other, their collision is not only considered when they physically hit one another, but also due to the interaction between their charges. In a region surrounding the two spherical charged particles develops an Electric field that affects the other approaching charges. For neutral species as well, the effective region in which any other species, if present, will collide with the target species because the radii of the two combined form a region in which the interaction is meant to occur. Therefore, the effective area of the interaction of the particles increases than their actual sizes.



### **2.10 NUCLEAR FUSION AND NEUTRON PRODUCTION**

In the chamber filled with energetic deuterium and tritium ions, the interactions and collisions lead to nuclear reactions with the two species combining to form helium gas and releasing neutrons in the process. The neutrons so released have high kinetic energies ranging from few keV to few MeV. The so obtained neutrons need to be

controlled. Thus the reaction can be allowed in safer regions with proper arrangements to harness the reaction products efficiently. Tokomak is one such example where the deuterium clusters undergo ion coulomb explosion. The ions can be restricted to some specific region of space by applying magnetic field. Higher the ion energy, lesser is the fusion energy that is released during the reaction.



$$D + T \xrightarrow{yields} He + {}_0^1n$$

Figure 9: Nuclear fusion and neutron formation Source: Google<sup>[26]</sup>

# Chapter 3

# **ION COULOMB EXPLOSION**

A femto-second laser pulse of Gaussian radial distribution of energy of the form

$$E_L = \hat{x}A(t, r, z)e^{-i(wt-kz)}$$

where,

$$A_{(z=0)}^{2} = A_{0}^{2}e^{-R^{2}/R_{0}^{2}}$$

is incident on the gaseous column of radius  $R_o$  containing clusters of deuterium gas, the sudden impact of a very high energy with a very short pulse ionizes the clusters. The radius of the laser pulse is same as the radius of the plasma cylinder. The electric field of the laser is strong enough to compete with the Coulomb field and strikes off the electron from the shells. We consider variable cluster density and the complete evacuation of the electrons from the clusters to study the Ion-Coulomb explosion in the following study. If we consider the partial evacuation, the inharmonic oscillations of the electrons over the cluster may lead to varying velocity and the varying electric field due to changing density also induces magnetic effects in the motion of the electrons. The remaining charged sphere undergoes fluctuations in hydrodynamic expansion and the Coulomb pressure and as the Coulomb pressure increases, the ions repel and move apart gaining energy. The excursion of the electrons is taken to be  $\Delta \sim 2r_c$ .

Let the atomic density of the deuterium gas is  $n_a$  which has a cluster density equal to  $n_c$ . Further each cluster has  $n_0$  atoms per unit volume. The radius of each cluster is well in the limits  $r_0 \ll c/\omega_p$  such that  $\omega_p = (4\pi n_0 e^2 / m)^{1/2}$  plasma frequency and c is the speed of light. The electrons are considered to leave the clusters for sufficient time then for the ions to explode. The intensity of the laser is given by  $I_L = \frac{\frac{1}{2\pi}m^2\omega^2r_o^2}{e^2}$ .

The divergence of the beam due to diffraction and nonlinearity in the plasma is however ignored and the plasma is considered to be formed within a few wave pulses only due to its high intensity and power. Therefore, after a certain number of pulses only the electrons completely leave the clusters <sup>[13]</sup>.

# 3.1 DENSITY VARIATION $\rho_0 = \rho_0 \left(1 - \frac{r^3}{r_o^3}\right)$

Considering a spherical distribution of positively charged deuterium ions of the mentioned charge variation, the electric field at a distance r from the center of the cluster can be calculated using the Gauss's law (eq. 2.2).

$$\frac{\mathrm{dq}}{\mathrm{dV}} = \rho$$

Therefore, dq=p.dV

In spherical coordinates,  $dV = r^2 dr d\theta d\phi$ 

Applying Gauss's Law to the sphere of radius r, (r < r0)

$$\oint \text{E.dr} = \left(\frac{1}{\epsilon_o}\right) \int dq$$

$$\text{E.}4\pi r^2 = \frac{1}{\epsilon_o} \int \rho \, dV$$

$$\text{E.}4\pi r^2 = \frac{1}{\epsilon_o} \int_0^r \rho_o \left(1 - \frac{r^3}{r_o^3}\right) dr \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi$$

Thus, the electric field at a distance r from the centre of the cluster turns out to be,

$$\mathbf{E} = \frac{\rho_0 r}{3\epsilon_0} \left( 1 - \frac{r^3}{2r_0^3} \right)$$
(eq.3.1)

Due to spherically symmetric distribution, i.e. only radial variation and no angular variations, the electric field is also only radial and varies as r.

Since the initial electric field varies directly as 'r', the force experienced by the ions at a larger radius would be greater as compared to the inner ions. Therefore, when the inner ions move outwards, the outer ions have already moved more away and therefore our assumption of the collision-less model of Ion-Coulomb explosion stands justified.

Now since all the electrons have left the cluster and only positive charge remains, the Ion Coulomb explosion occurs according to the obtained electric field.

Considering an ion initially at =  $r_i$ , electric field as seen by the ion is as

0.

dF

$$E_{i} = \frac{\frac{\rho_{o}}{3\epsilon_{o}}r_{i}^{3}}{r_{i}^{2}} \left(1 - \frac{r_{i}^{3}}{2r_{0}^{3}}\right)$$
(eq. 3.2)

Also,

And,

$$\frac{d^{2}t_{i}}{dr_{i}} = \frac{\rho_{0}}{3\epsilon_{0}} \left(1 - \frac{n_{1}}{2r_{0}^{3}}\right)$$
(eq. 3.3)  
$$\frac{d^{2}E_{i}}{dr_{i}^{2}} = -\frac{2\rho_{0}r_{i}^{2}}{\epsilon_{0}r_{0}^{3}} < 0$$
(eq. 3.4)

The equation (3.4) implies that the initial electric field experienced by the ions increases with the radius of the sphere under consideration. This is essentially due to the fact that more is the radius of the sphere, more is the charge enclosed inside it and increases the field.

 $4r^{3}$ 

Now, as the ions move away, the charge carried by the sphere of radius *ri* is moved to a new bigger sphere of radius r. the volume of the sphere increases but the charge remains the same. Thus, electric field experience b y the same ion which was initially at *ri* when moved to r is given by

$$E_r = \frac{\frac{\rho_o}{3\epsilon_o} r_i^3}{r^2} \left( 1 - \frac{r_i^3}{2r_0^3} \right)$$
 (eq. 3.5)

With increasing r, electric field decreases as  $r^2$ .

The equations (3.2), (3.4) and (3.5) together describe the movement of ions under the developed electric field. Initially, the ions experience a force given by eq. (3.2) which is greater for the ions at a larger distance from the centre of the cluster. But as the ions once start moving, the force experienced by them decreases with r as  $r^2$ .

Now, the energy gain by the ion in moving from *ri to r* is equal to the work done by the electric field on it. Using equation (2.1), we calculate the energy gain as:

$$\varepsilon_i = \int_{r_i}^r eE_r dr$$

$$\varepsilon_i = \frac{e\rho_o}{3\varepsilon_o} r_i^3 \left[ 1 - \frac{r_i^3}{2r_o^3} \right] \left[ \frac{1}{r_i} - \frac{1}{r} \right]$$
(eq. 3.6)

Now, let us consider that the ions move quite apart that they are under no more influence of each other, i.e.  $r \rightarrow \infty$  and also,  $\rho_o = n_o e$ 

$$\varepsilon_i = \frac{n_o e^2}{3\varepsilon_o} r_i^2 \left[ 1 - \frac{r_i^3}{2r_o^3} \right]$$
 (eq. 3.7)

This is a power 5 equation in *ri with respect to* E.

$$\frac{r_i^5}{2r_o^3} - r_i^2 + \frac{3\varepsilon_o}{n_o e^2} \varepsilon_i = 0$$
 (eq. 3.8)

The number of ions between the radiuses *ri and ri* + *dri* is given by the density of the states as (eq. 2.5). Therefore,

$$dN = 4\pi r_i^2 n_o \left[ 1 - \frac{r_i^3}{r_o^3} \right] dr_i$$

These ions will have the energy in the range  $\varepsilon_i \quad \varepsilon_i + d\varepsilon_i$ .

 $dN = 4\pi r_i^2 n_o \left(1 - \frac{r_i^3}{r_o^3}\right) \frac{dr_i}{d\varepsilon_i} d\varepsilon_i$  (eq. 3.9)

Now, from (eq.3.7), we find,

$$\frac{dr_i}{d\varepsilon_i} = \frac{3\varepsilon_o}{2n_o e^2 r_i \left[1 - \frac{5r_i^4}{4r_o^3}\right]}$$
(eq. 3.10)

substituting this equation back in (eq. 3.9) we obtain the number of ions as

$$dN = 2\pi r_i \left( 1 - \frac{r_i^3}{r_o^3} \right) \frac{3\varepsilon_o}{e^2 \left[ 1 - \frac{5r_i^4}{4r_o^3} \right]} d\varepsilon_i$$
 (eq. 3.11)

Therefore,

$$f(\varepsilon_i) = 2\pi r_i \left( 1 - \frac{r_i^3}{r_o^3} \right) \frac{3\varepsilon_o}{e^2 \left[ 1 - \frac{5r_i^4}{4r_o^3} \right]}$$
(eq. 3.12)

where  $f(\varepsilon_i)$  gives the ion energy distribution function from a single cluster.



### NEUTRON ESTIMATION

The number of neutrons for this density variation can also be calculated in the same manner as above.

The cumulative ion energy distribution function due to the Gaussian laser pulse can be evaluated by finding the number of clusters that ionize due to the pulse, i.e., the number of clusters that fall under the volume of the laser pulse.

$$F(\varepsilon) = \int_0^{R_0} f(\varepsilon) n_c 2\pi L R dR. d\varepsilon$$
$$F(\varepsilon) = \pi R_0^2 L n_c f(\varepsilon) d\varepsilon$$

During the fusion reactions, the number of neutrons produced will be half the number of fusion reactions.

No. of neutrons produced = 
$$\frac{No.of \ fusion \ reactions}{2}$$

$$N_{n} = \frac{N_{f}}{2}$$

$$N_{f} = L' n_{a} \int_{0}^{\varepsilon_{m}} F(\varepsilon) \sigma_{f} d\varepsilon = L' L \pi R_{0}^{2} \sigma_{f} n_{a} n_{c} \int_{0}^{\varepsilon_{m}} \frac{2 \pi r_{i} \left(1 - \frac{r_{i}^{3}}{r_{o}^{3}}\right) 3 \varepsilon_{o}}{e^{2} \left(1 - \frac{5r_{i}^{4}}{4r_{o}^{3}}\right)} d\varepsilon_{i}$$

Modifying the above energy integral in terms of the radial integral by changing the limits accordingly,

As 
$$\mathcal{E} = 0$$
,  $r_i = 0$  and  $\mathcal{E} = \varepsilon_m$ ,  $r_i = \sqrt{\frac{8}{9}}r_o$ 

$$N_{f} = L' L \pi R_{0}^{2} \sigma_{f} n_{a} n_{o} n_{c} \int_{0}^{\sqrt{\frac{8r_{o}}{9}}} 4\pi r_{i}^{2} \left(1 - \frac{r_{i}^{3}}{r_{o}^{3}}\right) dr_{i}$$

$$N_f = 2L'L\pi^2 R_0^2 n_a n_o n_c \sigma_f \left[\frac{r_i^3}{3} \left(1 - \frac{r_i^3}{2r_o^3}\right)\right]_0^{\sqrt{\frac{8n}{5}}}$$

The number of neutrons produced per Joule of energy,

$$n_{N} = \frac{\text{number of neutrons produce}d}{\text{total incident laser intensity}} = \frac{N_{n}}{I_{L}\tau_{L}\pi R_{o}^{2}}$$
$$n_{N} = \frac{2L'L\pi^{2}R_{o}^{2}n_{a}n_{o}n_{c}\sigma_{f} \left[\frac{r_{i}^{3}}{3}\left(1-\frac{r_{i}^{3}}{2r_{o}^{3}}\right)\right]_{0}^{\sqrt{\frac{8r_{o}}{9}}}}{I_{L}\tau_{L}}$$

Taking,  $L' = 100 \ \mu m$ ,  $L = 10 \ \mu m$ ,  $\sigma_f = 5 \times 10^{-28} cm^2$  (at 2.5 keV deuterium energy),  $r_o = 50 \times 10^{-8} cm$ , the intensity of the incident light for  $\Delta = 2 \ r_o$  is  $I_L = 3.2 \times 10^{16} W$  and  $\tau_L = 10^{-15} s$  and the values of  $n_a = 10^{19} cm^{-3}$ ,  $n_o = 10^{22} cm^{-3}$  and  $n_c = = 10^{17} cm^{-3}$ 

Putting the values of these

constants,  $n_N = 98125.3124 \sim 10^5 \frac{neutrons}{J}$ 

## **RESULT AND CONCLUSION**

Initial electric field experienced by ions varies directly with distance from the centre of sphere .As the ions starts moving ,the electric field decreases by  $r^2$ .

The energy variation can be expressed as apolynomial of degree 4 for the above taken density variation.

The expression for the ion energy distribution function  $f(\varepsilon)$ , is directly dependent on the initial radius of the ion.

The no of neutrons yielded are of order of  ${\sim}10^5 which gives us the estimation of fusion reactions made feasible .$ 

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