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CHARGING PROCESS OF A NANOPARTICLE IMMERSED INTO PLASMA CONSISTS (H+, H-, AND ELECTRONS)

عملية شحن جسيم قطره بالنانومتر مغمور في بلازما تتضمن (ايونات الهيدروجين الموجبة وايونات الهيدروجين السالبة والالكترونات)

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Abstract

This research presents a computer study to simulate of charging process for a nanoparticle (diameter =10 nm) immersed into plasma contain electrons, positive ions (H^+), and negative ions (H^-) (The mass of negative ion approximately equals to the mass of the positive ion), and studies statistical fluctuations of a nanoparticle charge with time. The research also appears effect of negative ion density on charge of nanoparticle.

الخلاصة

هذا البحث يمثل دراسة حاسوبيه لمحاكات عمليه شحن جسيم (قطره بحدود 10 نانومتر) مغمور في بلازما تحتوي ايونات الهيدروجين الموجب وايونات الهيدروجين السالب والالكترونات(كتله الايون السالب تقريبا مساويه لكتله الايون الموجب) لدراسة تغيرات شحنة الجسيم احصائي مع الزمن. هذا البحث أيضا يبين تأثير كثافة الايون السالب على شحنه الجسيم.

Introduction

In recent years, computer simulations studies are playing an important role in theoretical investigations in various branches of human activities. the situation is similar in the researches of negative ion plasma and nanotechnology, that is interesting not only for astronomers (interstellar clouds, comet tails etc.), but it found the place also in complicated technological processes like plasma etching of semiconductor devices. Recent in measurements of charged particles and plasma parameters in the nighttime polar mesosphere exhibited the presence of positively charged nanoparticles in the altitude range between 80 and 90 km, These positively charged particles were observed in a region dominated by positive and negative ions and very few electrons [1].

The space between the stars is filled with cosmic dust and elements like hydrogen and helium which make up the “interstellar medium”. The interstellar medium is mainly made of hydrogen atoms. The density of hydrogen in interstellar space is on average about 1 atom per cubic centimeter. In the extremes, as low as 0 .1 atom per cubic centimeter has been found in the space between the spiral arms and as high as 1000 atoms per cubic centimeter are known to exist near the galactic core [2].

Many of experiments and theoretical methods investigations have carried out for understanding the charging of dust particles in a plasma under different conditions [3, 4, 5]. The charge on the dust particle is not a constant, but can fluctuate randomly, or charge fluctuation on dust particle responses to plasma parameters such as the electron density, radius of dust particle, and the presence of negative ion in plasma. There are several experiments and some theoretical models to estimate the charge of a dust particle as well. However, none of them yields a result with perfect precision [4].

Su-Hyun Kim and Robert L. Merlino studied experimentally the effect of negative ions on the charging of dust particles in a plasma. A plasma containing a very low percentage of electrons is formed in a single-ended Q machine when SF6 is admitted into the vacuum system in 2006[5], and also in the same year, they studied experimentally charging of dust grains in a plasma with negative ions. When the relatively mobile electrons are attached to heavy negative ions, their tendency to charge the grains negatively is reduced. The grain charge can be reduced in magnitude nearly to zero ("decharging" or charge neutralization) [6].

E. I. Toader in his experiment shows that the possibility to use the reflex discharge plasma as a volume source of negative hydrogen ions [7].

Here we will consider theoretical model of charging which is known discrete model after it has developed. In general, the model is useful for estimating the charge with an accuracy of about a two factors time and density of negative ion in plasma. This model is also be useful for gaining a conceptual understanding of how the charge varies with plasma parameters, and how it can fluctuate in time. We investigate the charging of nanoparticle in plasma consisting of positive ions (H^+), electrons and negative ions (H^-) (for simplicity we refer to this as a negative hydrogen ion plasma).

Orbit Motion Limited (OML)

The Probe theories calculate the currents to an electrostatic probe as a function of probe potential and probe shape, The floating potential on probe is derived as the point where ions and electrons currents balance, First probe theories based on orbit motion limited (OML). Later, Probe theory has been applied to compute dust charging. Analytic OML model including:

1. The Dust Particle Charge:

The OML model typically assume that the particle is spherical shape, and its surface is an equipotential. In this case, even if the particle is not made of a conductive material, it can be modeled as a capacitor [4, 5]. The charge Q_d is then related to the particle's surface potential as, with respect to a plasma potential of zero, by

$$Q_d = 4\pi\varepsilon_\circ a\phi_s \quad \dots\dots \ (1)$$

Where a is the radius of the dust particle, and ϕ_s is the dust particle surface potential relative to the plasma potential. [6].

2. Currents to the Dust Particle:

For the collection of Maxwellian electrons and ions, characterized by temperatures T_e and T_i, the orbit-limited the electron and positive ion currents to the isolated spherical dust grain of radius (a) are given by[8,9]:

$$I_e = I_{eo} \times \begin{cases} 1 + \dfrac{e\phi_S}{kT_e} & \phi_s > 0 \\ e^{e\phi_S/kT_e} & \phi_s < 0 \end{cases} \quad \dots\dots \ (2)$$

$$I_+ = I_{+o} \times \begin{cases} e^{e\phi_S/kT_+} & \phi_s > 0 \\ 1 + \frac{e\phi_S}{kT_+} & \phi_s < 0 \end{cases} \quad \dots\dots \ (3)$$

The negative ion current participates in the charging of a dust grain in a plasma is [1]:

$$I_{-} = I_{-o} \times \begin{cases} 1 + \dfrac{e\phi_S}{kT_{-}} & \phi_s > 0 \\ e^{e\phi_S/kT_{-}} & \phi_s < 0 \end{cases} \quad \ldots\ldots..(4)$$

The coefficients I_{e0} , I_{-o} and I_{+0} represent the current that is collected for $\phi_s = 0$, and are given by

$$I_{jo} = q_j n_j \left(\frac{kT_j}{m_j}\right)^{1/2} 4\pi a^2 \qquad \ldots\ldots \quad (5)$$

Where $(j = e, -, or +)$

Particle Charging Models

There are some models, often implemented numerically to calculate the charge and potential of particle in a plasma, as described by Discrete Charging Model.

In this model, the electron and ion currents collected by the grain actually consist of individual electrons and ions. The charge on the grain is an integer multiple of the electron charge, $Q_d = Ne$, where N changes by -1 when an electron is collected and by +1 when positive ion is absorbed. Electrons and ions arrive at the particle's surface at random times, like shot noise. The charge on a particle will fluctuate in discrete steps (and at random times) about the steady-state value$\langle Q_d \rangle$ [4, 8].

There are two key aspects of the collection of discrete of plasma particles (we use the term "plasma particle" to refer to either electron or ions).

- First is that the time interval between the absorption of plasma particles (electrons and ions) varies randomly.
- Second is that the sequence in which electrons and ions arrive at the grain surface is random.

But neither of these is purely random; they obey probabilities that depend on the grain potential ϕ_s.

Let us define $p_e(\phi_s)$ and $p_i(\phi_s)$ as the probability per unit time for absorbing an electron or ion, respectively. As the grain potential becomes more positive, more ions will be repelled and more electrons will be attracted to the grain, so p_i should decrease with ϕ_s and p_e should increase. $p_j(\phi_s)$ (j refers to the ions, electrons) was calculated from the OML currents $I_j(\phi_s)$,

$$p_j = \frac{I_j}{q_j} \qquad \ldots\ldots\ldots (6)$$

This equation is the key to developing the discrete charging model. Basically, it converts the OML currents into probabilities per unit time of collecting particles. This relates the discrete charging model with its probabilities to the continuous charging model with its currents [8].

The total probability per unit time of collecting plasma particle is[8]

$$p_{tot} = \sum p_j \qquad \ldots\ldots\ldots\ldots (7)$$

The currents I_j depend on the grain surface potentialϕ_s, so p_{tot} also depends on ϕ_s and hence on charge Q_d .

Development of the Discrete Model

The discrete model was developed to include effect of negative ion on the charging process of dust grain in a plasma negative ion instead of plasma electron-ion [10]. The model is useful for gaining a conceptual understanding of how the charge varies with plasma negative ion parameters, and how it can vary in time. Which in general is useful for estimating the charge of dust grain.

The model has described the charging process of an isolated dust grain immersed in a negative ion plasma and assumed a spherical grain with radius a which initially uncharged under the condition $a \ll \lambda_d \ll \lambda_{mfp}$, where a is the particle radius, $\lambda_d$is length, and ,$\lambda_{mfp}$is a collisional mean-free-path between neutral gas atoms and either electrons or ions In this case. The charging process is characterized by [10]:

1. It is based on the assumption that the plasma particles arrive to dust surface at random time intervals Δt_j , which is not fixed
2. The probabilities of arriving electrons or ions (negative or positive) in equations (6) depend on the surface potential of the dust grain.
3. The total probability per unit time of collecting plasma particle is calculated from equation (7)
4. The time interval Δt_j depends on the potential of the grain surface $\phi_s$and the random number R_1 that was generated.
5. The discrete model assumes that plasma particles arrive in a random sequence in consistent with the probabilities.
6. To recognize the plasma particle type electron or ion (negative or positive), it must compare the probability $\mathrm{P_j/P_{tot}}$ with another random number R_2.
7. The charge Q_d of the dust would be changed after each electron or ion (negative or positive) collection, and it is increased or decreased by one charge.
   The simulation converts the physical discrete charging model after add negative ions current to program which simulates the charging process of a dust grain immersed in plasma with negative ion.

At first the dust grain would be uncharged so the computer experiment starts with a zero charge $Q_\mathrm{j} = 0$ at a time step equal zero $t_\mathrm{j} = 0$ where j refers to plasma particle electron, negative ion or positive ion, then two steps will be repeated for plasma particles which will fall on the dust.

A. First Step: The Random Time Intervals

This step is based on the physical discrete charging model, which assumes that the plasma particles arrive at random time intervals, there will be one time step per particle that is collected and it corresponds to:

$\Delta t_j = t_j - t_{j-1}$ …………….. (8)

The currents I_e, I_- and I_+ must calculated from equations (2, 3, and 4) there are predicted by the OML theory to find the probabilities.

The random time step Δt_j depends on the probability per unit time of collecting a plasma particle $P_e(\phi_s)$,$P_-(\phi_s)$, $P_+(\phi_s)$ and the total probability is given in equation (7)

The probability of collecting a plasma particle is [8]:

$P = 1 - exp(-\Delta t_j . P_{tot})$ ………….. (9)

To calculate the random time interval one must generate a random number R_1 where $0 \le R_1 \le 1$ and equate it to the previous equation of probability to yield [8]:

$\Delta t_j = -\,ln(1 - R_1)\,/P_{tot}$ …….. (10)

B. Second Step: The type of plasma particle

The plasma particle arrives in a random sequence. Generate a random number R_2 to determine whether the next collected particle is an electron or an ion (negative or positive), where $0 < R_2 < 1$.

Probability of the next particle (electron, negative ion or positive ion) equals to $= \mathrm{P_j/P_{tot}}$ and compares with R_2 as follows [10]:

i. If $R_2 < \mathrm{P_e/P_{tot}}$ then the charge will be $Q_j = Q_{j-1} - e$ that means the process is electron collection. However, at state $R_2 > P_e/P_{tot}$that means the process isn’t electron collection. The probability of other particle must examined.

ii. If $\mathrm{R_2} < P_-/\mathrm{P_{tot}}$ then the charge will be $Q_j = Q_{j-1} - e\, z_{ni}$ that means the process is negative ion collection.

iii. If $R_2 > P_-/P_{tot}$ then the charge will be $Q_j = Q_{j-1} + e\, z_{pi}$ that means the process is positive ion collection.

Programing of The model

After the discrete charging model was developed, that was translated to numerical calculations using computer program. The program was written in FORTRAN language to simulate a computer experiment of the charging process for a dust grain in negative ion plasma. The program computed statistical calculations such as the time distribution of a dust charge, equilibrium charge and charging time for different value of η_e(ratio of number density of electron to number density of positive ion)[10]. In this research, we can apply this model on nanoparticle that immersed into plasma. This plasma contains electrons, positive ions (H^+), and negative ions (H^-) (The negative ions have a mass approximately equal to the mass of the positive ion).

Results and Discussion

The results of program are a sequence of the calculations process, which is done as the following steps:

1. The charge fluctuations on nanoparticle

Calculations show the charge number (*N*) on nanoparticle (the charge on the nanoparticle is an integer multiple of the electron charge, $Q_d = Ne$) fluctuates with time. when nanoparticle with diameter = 10nm immersed in H^+ plasma if a significant fraction of the electrons are attached to negative ions; the magnitude of the charge on the nanoparticles is reduced. The ions and electrons have equal temperatures $T^+ = Te = T^- = 0.2$ eV.

For comparison purpose, we will study charging process of nanoparticle immersed into plasma consists electrons and positive hydrogen ion. The presence of the particle with diameter = 10nm in this plasma (e-H^+ ion) leads to charging the particle negatively because the mobility of electrons larger than mobility of ions .The charge on the grain will reach the equilibrium state in which the charge Q will fluctuate around the equilibrium charge<Q>. Figure(1) showes the chraging process for a nanoparticle by collecting electrons, and positive ions from plasma with out negative ion,notes that the range of the charg fluctutions between zero and-7.

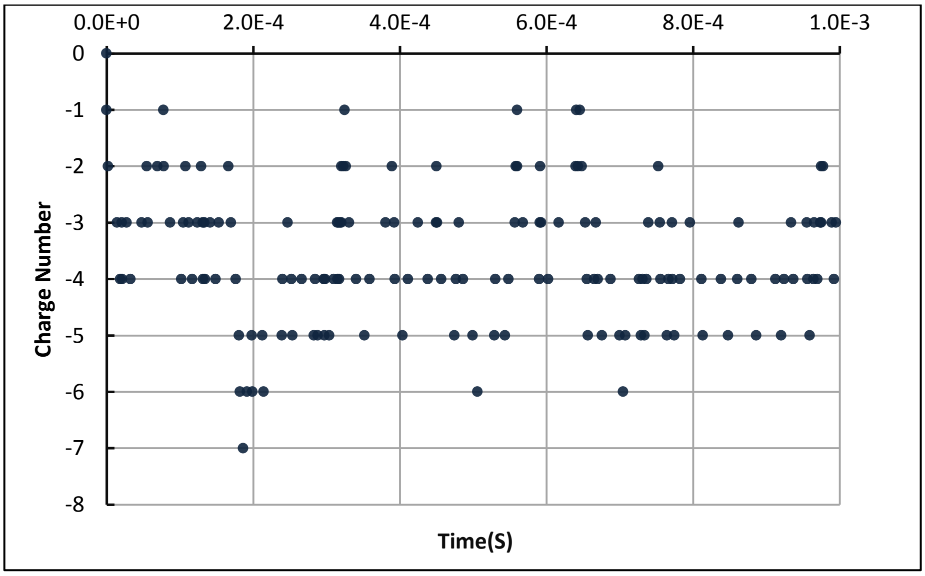


Figure (1): Charge number on surface of nanoparticle as a function time when diameter of particle=10nm, ηe =1 (no negative ion)

Negative ion plasma is formed by Dissociative attachment from vibrational excited H_2 molecules in their ground electronic state is the main accepted mechanism for H^- negative-ion production in volume plasmas. This process can be described as [7]

$$e_{slow} + H_2^* \rightarrow H + H^-$$

When the H^-density is created in H^+ plasma. There is a corresponding reduction in the electrons current due to some electrons become attached to form H^- ions, as Figure (2) shows that the range of the charge fluctutions is between 1 and -4 and the renge drifts toward positive compare with Figure (1).

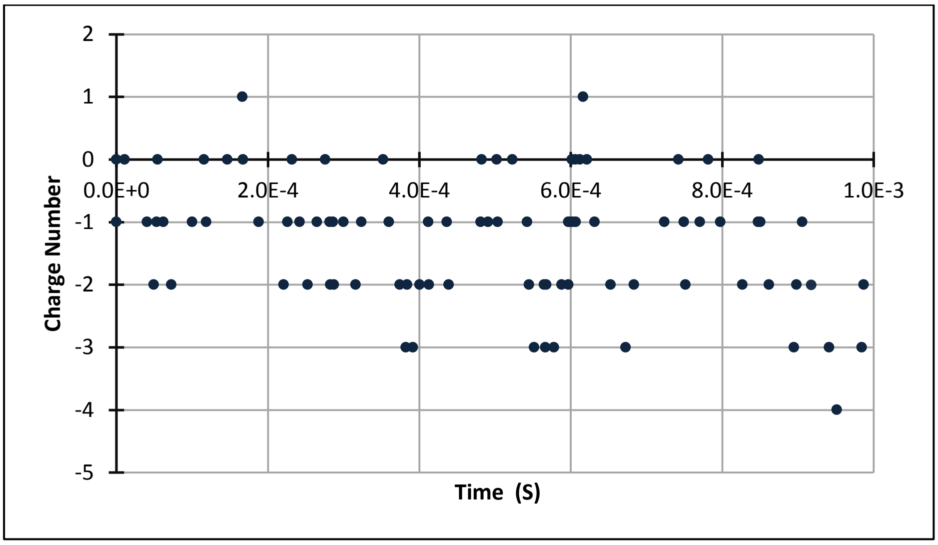


Figure (2): Charge number on surface of nanoparticle as a function time when diameter of particle =10nm, $\eta_e=10^{-1}$.

When the H^-density is increased in H^+ plasma, more electrons become attached to form H^+ ions. Therefore, the negativity of charge number on nanoparticle decreases gradually. Figures (3), and (4) show that the range of the charge fluctuations both of them is about (-1, 1).

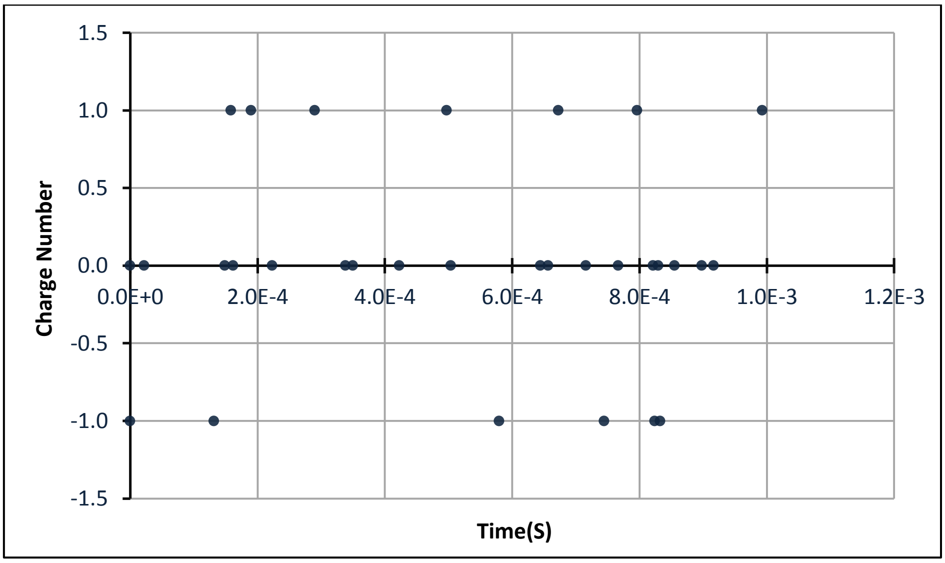


Figure (3): Charge number on surface of nanoparticle as a function time when diameter of particle =10nm, $\eta_e=10^{-2}$

2. **The Time Distribution of The grain Charge**

After the collection of charges by nanoparticle, these charges will approach the equilibrium value <Q> and the probabilities for collecting electrons, negative ions(H^-), and positive ions(H^+) are unequal so the charge will always fluctuate around the equilibrium value. The charge distributions are determined from the time series by making histogram of time spent at each charge level to calculate charge equilibrium value, the equilibrium charge number takes larger time from computer experiment time. Figures (5), (6), (7), and (8) show distribution functions for each case in the previous section.

In figure (5) the chraging process for a nanoparticle by collecting electrons and positive ions (H^+) from plasma. Positive ions (H^+) are much heavier than electrons therefor the nanoparticle becomes negatively charged. The equilibrium charge number is -4 because this level takes longer time in comparison with other levels.

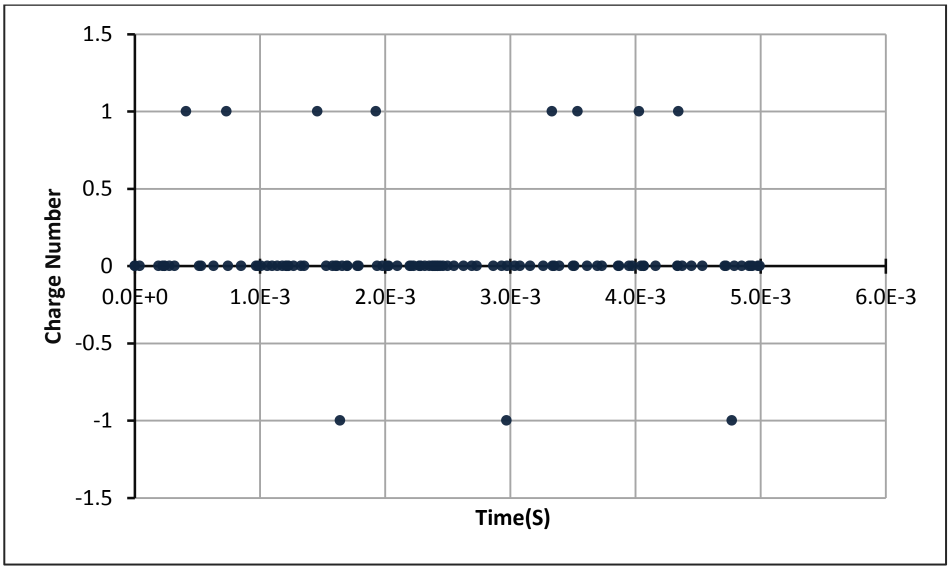


Figure (4): Charge number on surface of nanoparticle as a function time when diameter of particle =10nm, η_e=10^{-3}

When the H_2^*density is created in H^+ plasma, some electrons become attached to form H^- ions and η_e=10^{-1}, the negativity of charge number on nanoparticle decreases and the equilibrium charge number becomes -1. Figure (6) shows that.

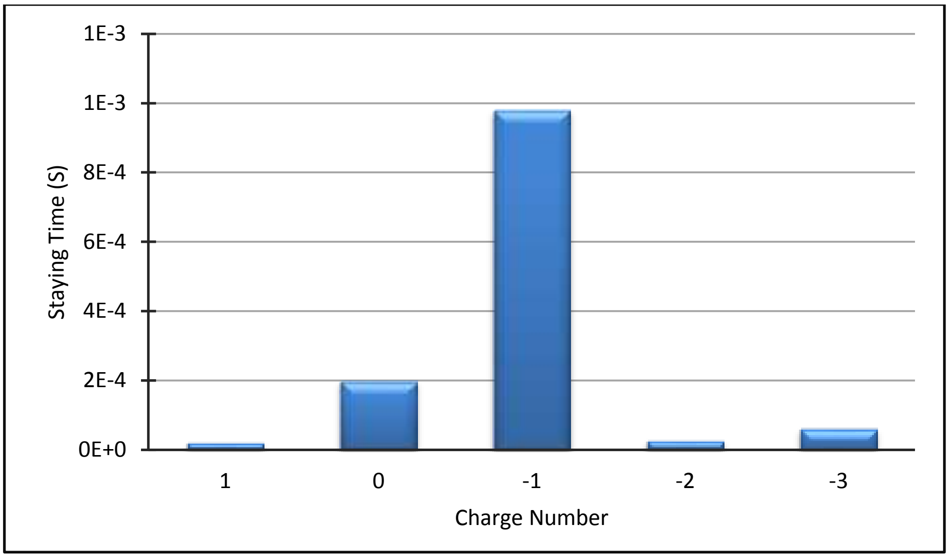


Figure (6): Charge distribution function for nanoparticle of diameter=10nm, $\eta_e=10^{-1}$. The equilibrium charge number is=-1

If the H_2^* density is increased in H^+ plasma so as to $\eta_e=10^{-2}$, the equilibrium charge number becomes zero as in the figure (7).

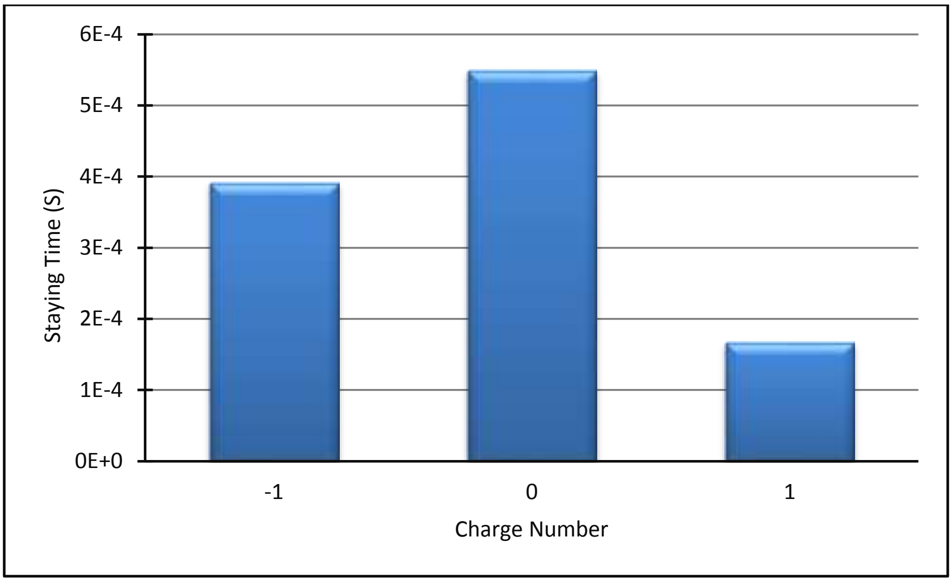


Figure (7): Charge distribution function for nanoparticle of diameter=10nm, $\eta_e=10^{-2}$. The equilibrium charge number is=0.

When the ratio of number density of electrons to number density of positive ions equals 10^{-3}. The charge number on dust grain becomes constant and equals zero that means the positive ions current and the negative ions current dominates on charging process of nanoparticle and probability of negative ions to arrive nanoparticle surface equal to probability of positive ions. Because, the negative ions have a mass approximately equal to the mass of the positive ion and number density of electrons is sufficiently small. Figure (8) shows that.

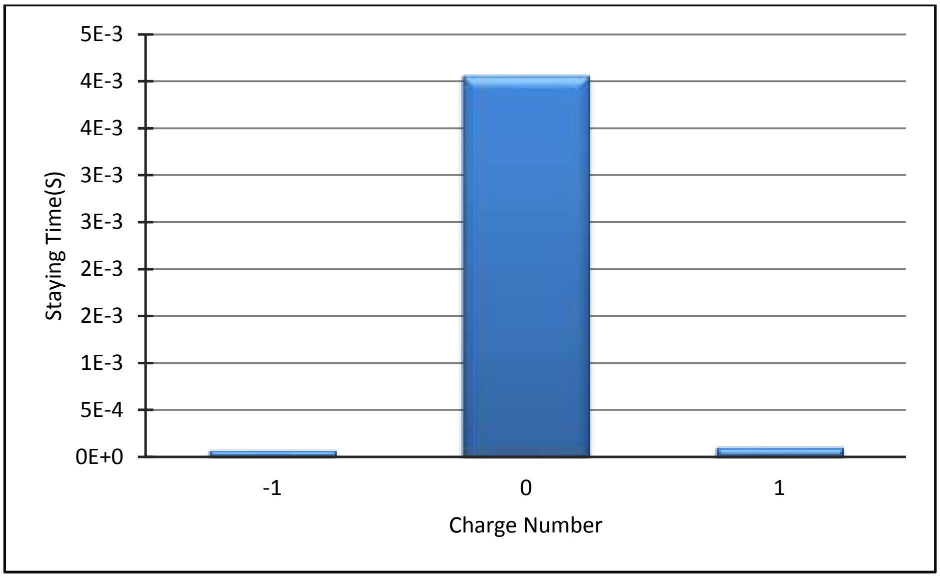
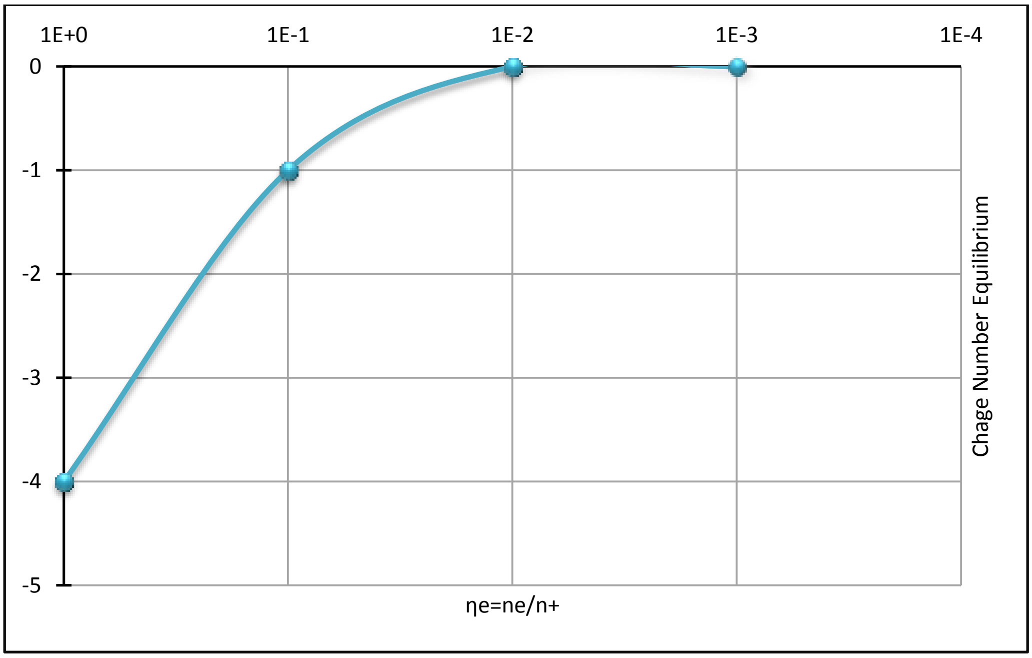


Figure (8): Charge distribution function for grain of diameter=10nm, $\eta_e=10^{-3}$. The equilibrium charge number is=0.

3. The Equilibrium Charge Number

The charges on nanoparticle approach the equilibrium value $\langle Q \rangle$, after the collection of charges by nanoparticle, The charge on nanoparticle will fluctuate in discrete steps (and at random times) about the steady-state value$\langle Q \rangle$.

A plot of the equilibrium charge number on nanoparticle (N) as a function for the parameter $\eta_e = n_e / n_+$ for the case in which the positive ion is hydrogen H^+ and the negative ion is H^- is shown in figure (9) for nanoparticle diameter equals 10nm. Notice that the negative charge on the nanoparticle surface is reduced gradually and became constant at zero.



Figure(9): the equilibrium charge Number of nanoparticle (diameter=10nm) as a function of the parameter ηe

Conclusions

The charging of nanoparticle in plasma contains electrons, positive ions (H^+), and negative ions (H^-) (The negative ions has a mass approximately equal to the mass of the positive ion) can be controlled by varying the relative fraction of negative ions in the plasma. When the negative ion density increases, the relatively mobile electrons are attached to negative ions the magnitude of the negative nanoparticle charge is reduced and became constant equal to zero.

The charge equilibrium value calculates from the time series by making histogram of time spent at each charge level. Where, the charge distribution function has peak at the equilibrium charge value.

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