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EFFEC TIVE SHORT RANGE COULOMB INTERACTION IN ION DYNAMICS

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1. Introduction

The kinetics of a system composed of charged particles may be described by the Boltzmann Equation, which may be written using a mean field approximation [1]. The mean electric field results from the distribution of the charged particles. The Boltzmann collision operator gives the rate of change of the phase space configuration of the particles caused by the collisions. This operator is defined in terms of the kind of the interaction (responsible for the scattering), the impact parameter, the initial and the outgoing particles velocities and the angle of scattering.

The Boltzmann equation is adequate for dilute systems composed of particles interacting through a short range potential, i.e., the range of interaction is small if compared to the average distance between particles. However, for Coulomb potential the range of interaction is not finite and so the condition cannot be satisfied. Many methods have been developed for deriving a kinetic equation for systems with Coulomb interaction such as in [1, 2].

This work proposes a novel form to deal with Coulomb collisions in ion dynamics using an effective interaction which provides a correction to the mean electric field approach. This effective interaction is a short range interaction, that can be used for defining the Boltzmann collision operator.

2. Mean field correction

The mean field obtained from a distribution of charged particles that interact through a Coulomb potential would correspond to the exact electric field if all the particles (and so their charge) could be uniformly distributed in the space and, at the same time, letting the local density unchanged. The electric field in a position $\mathbf{r}$ resulted from a distribution of N particles with positive electrical charge e, each one in position $\mathbf{r}_j$, is

$$\mathbf{E}(\mathbf{r}) = e\sum_{j=1}^{N}\frac{\mathbf{r}-\mathbf{r}_j}{\left\|\mathbf{r}-\mathbf{r}_j\right\|^3}\,. \tag{1}$$

On the other hand, for a corresponding smoothed distribution with continuous density $\rho(\mathbf{r})$, the electric field will be

$$\mathbf{E}(\mathbf{r}) = e\int\frac{\mathbf{r}-\mathbf{r}_1}{\left\|\mathbf{r}-\mathbf{r}_1\right\|^3}\rho(\mathbf{r}_1)dr_1^3\,. \tag{2}$$

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Analyzing the difference between these two electric fields one can see that the system composed by the point charge particles would be similar to the continuous representation if the charge and the mass of each particle could be spread over its corresponding proper volume Ω = $1/\rho$. Following this reasoning, it is assumed that in an arbitrary position $\mathbf{r}$ the electric field $\mathbf{E}(\mathbf{r})$ for the continuous distribution will be different from the discrete distribution just for particles closer than $\Omega^{1/3}$ from the position $\mathbf{r}$. Thus the distance $R = \Omega^{1/3}$ may be seen as a range of an effective interaction where a correction in the mean electric field must be done. In order to justify this assertion it is enough to compare the electric field generated by a point charge with the electric field generated by a continuous and homogeneous density charge inside a sphere of radius $R = \Omega^{1/3}$. The electric field of a point particle of charge e is

$$\mathbf{E}(\mathbf{r}) = e\mathbf{r} / r^3 , \tag{3}$$

The field of a homogeneous and spherical charge distribution with radius R is given by

$$\mathbf{E}_s(\mathbf{r}) = \begin{cases} e\mathbf{r}/R^3, \text{ for } r < R; \\ e\mathbf{r}/r^3, \text{ for } r \geq R. \end{cases} \tag{4}$$

Then the difference between these two fields is given by

$$\delta\mathbf{E}(\mathbf{r}) = \mathbf{E}(\mathbf{r}) - \mathbf{E}_s(\mathbf{r}) = \begin{cases} e(1/r^3 - 1/R^3), \text{ for } r < R; \\ 0, \text{ for } r \geq R. \end{cases} \tag{5}$$

It is possible to observe that $\delta\mathbf{E}(\mathbf{r})$ is a mean field correction that corresponds to a binary interaction with range R, so it is a short range interaction. The interaction $\delta\mathbf{E}(\mathbf{r})$, which is called effective Coulomb interaction, consists on a correction that must be added to the mean electrical field applied to a point particle.

Note however, that the field $\delta\mathbf{E}(\mathbf{r})$ will be the exact mean field correction just if the variation of the mean field within the proper volume $\Omega = 1/\rho$ is negligible. Of course that this variation does not correspond to the deviations of the field $\mathbf{E}(\mathbf{r})$ caused by the charged particles placed closer than a distance $\Omega^{1/3}$ from $\mathbf{r}$, because such a deviation is the one that the field $\delta\mathbf{E}(\mathbf{r})$ is supposed to correct. Note that the effective interaction is dependent on the particles density since that $R^3(\mathbf{r},t) = 1/\rho(\mathbf{r},t)$.

3. Scattering cross section

The potential energy for the effective interaction, obtained from (5), is given by

$$U_{ef}(r) = \begin{cases} \mathrm{e}^2\left(\dfrac{1}{r} + \dfrac{r^2}{2R^3} - \dfrac{3}{2R}\right), \text{ for } r \leq R; \\ 0, \text{ for } r > R. \end{cases} \tag{7}$$

The scattering cross section that results from the effective two body interaction $\delta\mathbf{E}(\mathbf{r})$ may be deduced following the method presented in [1], which provides the following relation between the total energy of the system described in the center of mass of the two particles (H_{cm}), the scattering angle (θ) and the impact parameter (b):

$$\theta(R,b,H) = \int_{b/R}^{x_0} \frac{dx}{\sqrt{1-x^2-\dfrac{e^2}{H_{cm}b}\left(x+\dfrac{1}{2x^2}(b/R)^3-\dfrac{3b}{2R}\right)}} + \int_{b/R}^{x_0} \frac{dx}{\sqrt{1-x^2}}. \qquad (8)$$

where x is equal to b/r and r is the distance from the origin (i.e. the center of mass of the two particles).

Equation (8) may be used for calculating the Boltzmann scattering operator since it allows relating the velocities of the particles before collision with the outgoing velocities.

4. Simple numerical results

Some results of the effective Coulomb interaction are presented for a deuteron field with conditions typically found in inertial electrostatic confinement devices (IEC) [3, 4]. Figure (1) shows the angle of deviation ($\varphi = \pi - 2\theta$) as function of the square of the impact parameter normalized by the range of interaction.

For the range of energy and density analyzed most part of the scattering cross section, of particles interacting through the effective interaction is related to small angle of deviations which implies a small energy transfer between the particles. For case (a) the probability of deviation of an angle less than 0.005º in the collision process is greater than 80 %; for the conditions of case (b) there is a probability higher than 95% for the angle of deviation to be less than 10^{-4} degrees when a collision takes place; and for the conditions of case (c) more than 99% of the total cross section is related to a deviation angle less than $2\text{x}10^{-6}$ degrees.

For the conditions of case (b) the impact parameter for onset of fusion in a deuteron-deuteron collision is about $7.3\text{x}10^{-7}$nm [5]. This impact parameter is calculated as $b = \sqrt{\sigma/\pi}$, where σ is the microscopic cross section for fusion. From Fig. (1d) it is possible to compare the scattering cross section with the fusion cross section. The region where the probability of fusion is appreciable in a deuteron-deuteron collision varies from a frontal collision, φ = 180º to approximately φ = 169º.

From the results shown it can be seen that a decrease in density or an increase in energy cause an increase of the fraction of the scattering cross section related to small angle of deviation.

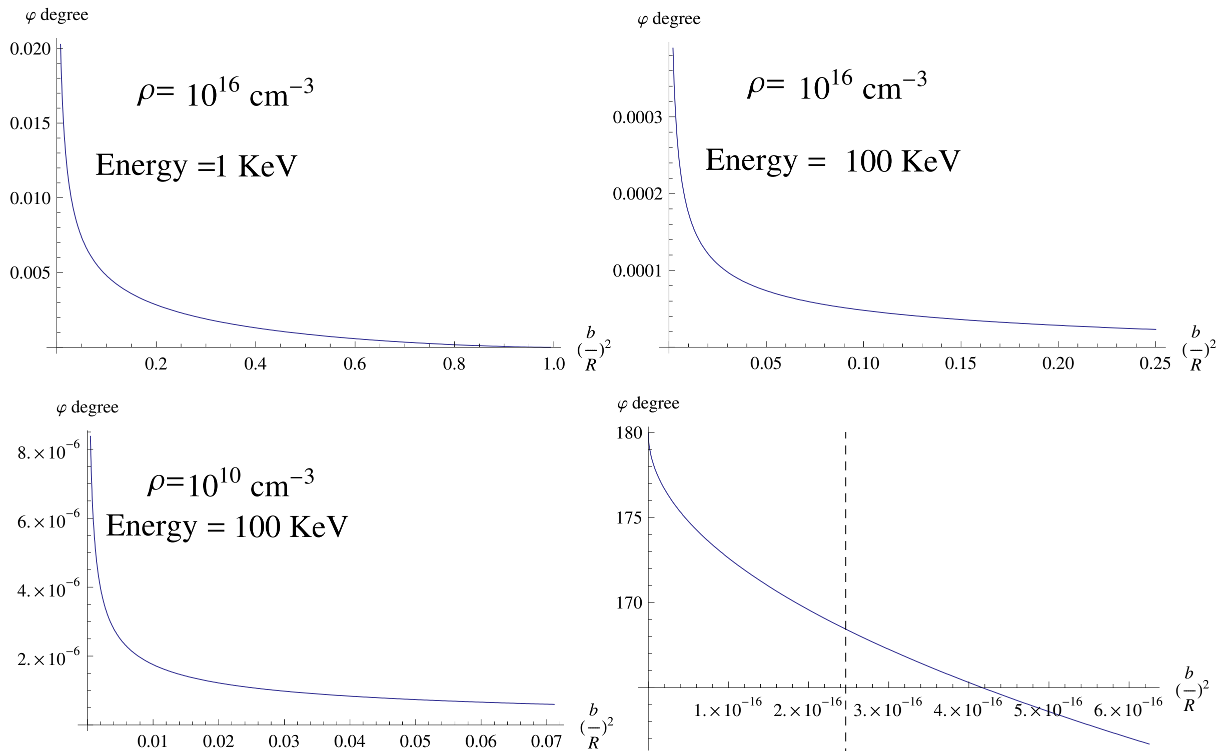

Figure 1. Deviation angle (φ) as function (*b*/*R*). (a) Energy 1KeV and density 10^{16} cm^{-3}; (b) energy 100KeV and density 10^{16} cm^{-3}; (c) energy 100KeV and density 10^{10} cm^{-3}; (d) same conditions of (b) showing the region of the onset of the deuteron-deuteron fusion reaction (the vertical dashed line indicates the onset of fusion).

5. Conclusion

In this work a novel method to deal with Coulomb collision in ions dynamics is developed. This model provides a correction to the mean electric field approach, transforming the long range Coulomb interaction into a short range interaction. The cross section for the short range Coulomb interaction is calculated and analyzed for some characteristic conditions of IEC devices.

This model can be used to obtain an expression for the Boltzmann collision operator allowing calculating more realistic ion phase-space distribution in several situations of interest. It is now is underway a study to use the effective interaction together with a Boltzmann type equation to describe the time evolution of the energy and angular momentum distribution of ions in an IEC device.

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