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EFFECTIVE SHORT RANGE COULOMB INTERACTION IN ION DYNAMICS

F. Paolini, E. L. L. Cabral, A. dos Santos

Abstract. A short range effective interaction is developed to be used as a correction to the electric mean field dynamics of a system of charged particles. It allows the direct application of the Boltzmann collision operator to the ion dynamics. The details of an explicity calculation is left to a second work.

1. Introduction

The kinetics of a system composed of charged particles may be described by the Boltzmann Equation [1], which may be written as an addition to the mean field approximation [2] of the electric field which results from the distribution of the charged particles. The Boltzmann collision operator gives the rate of change of the phase space configuration. This operator is characterized by the details of the binary interaction (responsible for the scattering), and usually evolves the phase space distribution to thermal distribution.

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, the range of the Coulomb potential 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 [2, 3, 4]. This work proposes a novel form to deal with Coulomb collisions in ion dynamics, through the use of a short range effective interaction, which may be used to build a Boltzmann collision operator and so providing a correction to the mean electric field approach.

2. Mean field correction

The mean field obtained from a distribution of charged particles that interact through the 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 macroscopic density unchanged.

The electric field in a position $\mathbf{r}$ resulting from a distribution of N particles with positive electrical charge e, each one in the position $\mathbf{r}_j$, is

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

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On the other hand, for a corresponding smoothed distribution with continuous density (**r**), the electric field will be

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

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/ . Following this reasoning and being helped by the Gauss law of electrostatic, it is assumed that in an arbitrary position **r** the electric field **E**(**r**) for the continuous distribution will be different from the discrete distribution (the exact one) just due particles closer than $\Omega^{1/3}$ from the position **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 of charge inside a sphere of radius $R = \Omega^{1/3}$ and with the same total charge. 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

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

The difference between these two fields is given by

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

It is possible to consider **E**(**r**) as an effective Coulomb interaction of range R, that may be included to correct the mean field approach. Thus the dynamics of the charged particles may be improved if written in terms of the mean field added of **E**(**r**). However, the field **E**(**r**) will be the exact mean field correction just if the variation of the mean field within the proper volume Ω = 1/ is negligible, because the procedure described above provides the correction of the field applied to a punctual particle, while the mean field spreads this particle evenly over the whole proper volume. At last it is worth noticing that the effective interaction is dependent on the particles density, since $R^3(\mathbf{r},t) = 1/\;(\mathbf{r},t)$, which turns the calculation more difficult.

3. Scattering cross section

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

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

The scattering cross section that results from the effective two body interaction **E**(**r**) may be deduced following the method given in [1], which provides a relation between the total energy of the binary system described in the center of mass frame system (H_{cm}), the scattering angle ( ) and the impact parameter (b):

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

where x is equal to b/r and r is the relative distance between the two particles. The eq. (8) may be used to calculate 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) [6, 7]. Figure (1) shows the angle of deviation (= − 2) as function of the square of the impact parameter normalized by the range of interaction $(b/R)^2$.

For the range of energy and density analyzed, most part of the scattering cross section 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 $b = \sqrt{\ \ /\ \ }$, where   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,   = 180º to approximately   = 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 deviation.

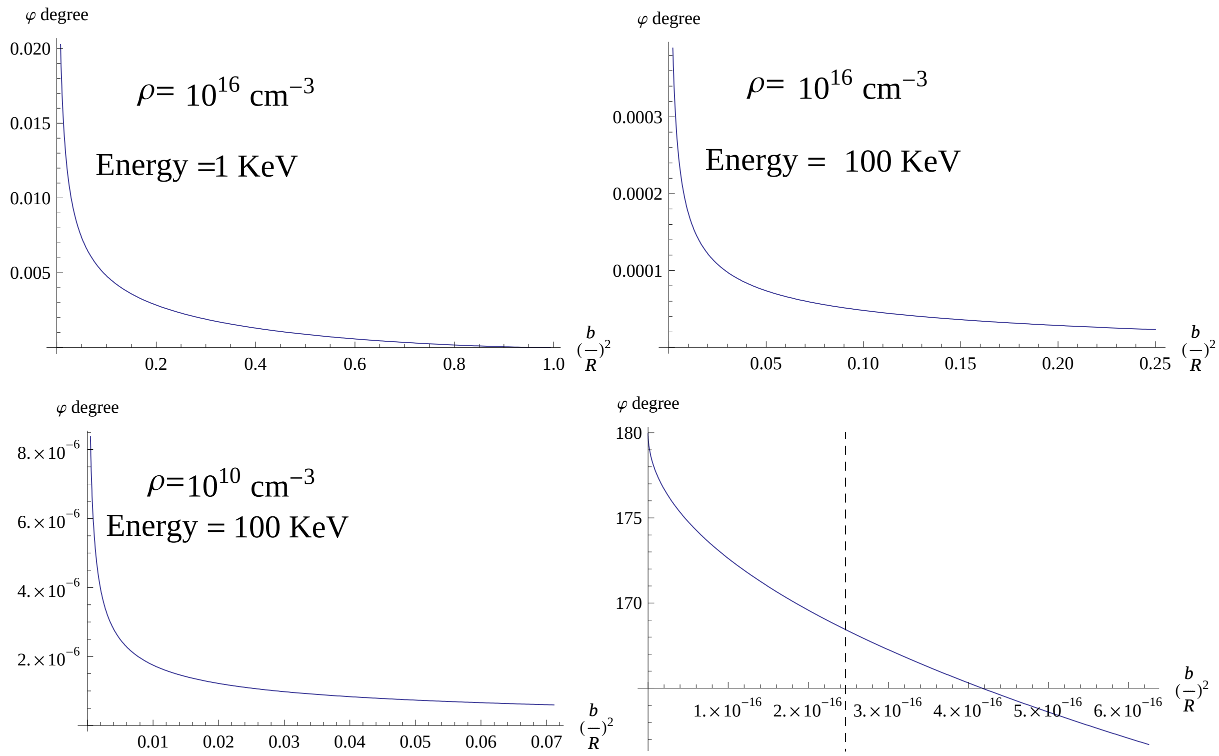

Figure 1. Deviation angle ( ) as function (*b*/*R*). (a) Energy 1KeV and density 10^{16} cm^{-3}; (b) energy 100KeV and density 10^{16} cm^{-3}; (c) energy 100KeV and density 10^{10} cm^{-3}; (d) same conditions of (b) showing the region of the onset of the deuteron-deuteron fusion reaction (the vertical 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 problem into a short range one. 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 to calculate more realistic ion phase-space distribution in several situations of interest. It is now in underway a study to use the effective interaction together with a Boltzmann type equation to describe the dynamics of the phase space of ions in an IEC device.

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