Time-average and ergodic methods for the dynamics of electron plasmas

G. COPPA(1)(*), A. D’ANGOLA(2) and R. MULAS(1)

(1) Politecnico di Torino - corso Duca degli Abruzzi 24, 10129 Torino, Italy
(2) Università della Basilicata - via dell’Ateneo Lucano 10, 85100 Potenza, Italy

SUMMARY. — The paper deals with the dynamics of electrons confined by a two-dimensional electrostatic field and by a constant magnetic field. The electrons undergo collisions with neutral atoms, with frequency much smaller with respect to the characteristic frequencies of the motion. In this situation, suitable time averages of the trajectories can be introduced in order to simplify the analysis of the problem. Two different approaches are described: 1) the time average of the trajectories and 2) the use of a suitable ergodic distribution. Results obtained with the two methods are presented and discussed.

PACS 52.25.Dg – Plasma kinetic equations.
PACS 52.27.Jt – Nonneutral plasmas.
PACS 52.65.Pp – Monte Carlo methods.

1. – Introduction

In a previous work [1], some of the Authors studied the dynamics of the expansion of spherical plasmas using a new method based on the time average of the trajectories, instead of following exactly the electron motion; moreover, these averages were calculated by using an ergodic distribution for each particle (a discussion on the validity of the method is reported in [2]). Comparisons with reference numerical simulations demonstrated that the method provides accurate results in terms of energy spectrum and space density distribution. For this reason, a similar technique is here proposed to study the dynamics of an electron plasma [3, 4] in the presence of collisions with neutral atoms. The final purpose of the research is investigating the effect of a very low-pressure gas inside a Penning trap [3] used to confine an electron plasma. To show the effectiveness of the method, a simple two-dimensional problem is considered, in which the electrostatic potential (generated by the electrodes) is proportional to \( y^2 - x^2 \) and the self-consistent
field is negligible. In addition, a constant magnetic field in $y$ direction is present. In this case, the canonical momentum $p_z$ is a constant of the motion and in the $(x, y)$ domain the particles move according to an effective potential $U(x, y) = U_x(x) + U_y(y) + \text{const}$; as the motion is a simple composition of two oscillators along $x$ and $y$ directions, to each electron can be associated a phase-space distribution depending on three parameters $\{p_z, \epsilon_x, \epsilon_y\}$, where $\epsilon_x$ and $\epsilon_y$ represent the energies for the motion along $x$ and $y$ directions. Alternatively, a simplified “ergodic” model can be used, in which to each particle is associated the distribution $\delta\left[\frac{m}{2}(v_x^2 + v_y^2) + U(x, y) - \epsilon\right]$, $\epsilon$ being the total energy.

The assumption is rigorously correct in the presence of perturbations of the potential, otherwise it represents a simplified description of the real physical system. In the last section of the paper, results obtained with the two different approaches are presented and discussed.

2. – Properties of the motion of the electrons

Between two successive collisions, the motion of a particle of charge $q$ is governed by the equations

\[
\begin{align*}
\frac{dv_x}{dt} &= -\frac{q}{m} \frac{\partial \Phi}{\partial x} - \omega_c v_z, \\
\frac{dv_y}{dt} &= -\frac{q}{m} \frac{\partial \Phi}{\partial y}, \\
\frac{dv_z}{dt} &= \omega_c v_x,
\end{align*}
\]

(1)

where $\omega_c = qB/(mc)$ is the Larmor frequency and $\Phi(x, y)$ is the electrostatic potential. From the third equation (1), one obtains immediately $v_z = \omega_c x + \text{const}$, which states that the canonical momentum

\[
p_z = m(v_z - \omega_c x)
\]

(2)

is a constant of the motion. Therefore $v_z$ can be eliminated from the first equation (1) and the equations of the motion in the $(x, y)$-plane can be written as

\[
\begin{align*}
\frac{dp_x}{dt} &= -q \frac{\partial \Phi}{\partial x} - m\omega_c (\omega_c x + p_z/m), \\
\frac{dp_y}{dt} &= -q \frac{\partial \Phi}{\partial y} .
\end{align*}
\]

(3)

By defining the effective potential, $\mathcal{U}$, as

\[
\mathcal{U}(x, y) = q\Phi(x, y) + \frac{1}{2m} (m\omega_c x + p_z)^2,
\]

(4)

the equations of the motion can be deduced from the Hamiltonian

\[
\mathcal{H}(x, y, p_x, p_y) = \frac{1}{2m} \left( p_x^2 + p_y^2 \right) + \mathcal{U}(x, y) = \\
= \frac{1}{2m} \left[ p_x^2 + p_y^2 + (m\omega_c x + p_z)^2 \right] + q\Phi(x, y).
\]

(5)
As $\mathcal{H}$ does not depend explicitly on time, its value is a constant of the motion:

$$\mathcal{H} (x(t), y(t), p_x(t), p_y(t)) = \text{const} = \epsilon$$

and it coincides with the total energy of the electron in the potential field $\Phi$. The level curves for $\mathcal{U}(x, y)$ and $\Phi(x, y)$ have the following property: given a generic point $(x_0, y_0)$, if $p_z = -m\omega_c x_0$, then the two curves $\Phi(x, y) = \Phi(x_0, y_0)$ and $\mathcal{U}(x, y) = \mathcal{q}\Phi(x_0, y_0)$ are tangent in $(x_0, y_0)$. In fact, the tangent line to $\Phi = \text{const}$ is such that $d\Phi = 0$ and so $\frac{\partial \Phi}{\partial x} dx + \frac{\partial \Phi}{\partial y} dy = 0$, while the tangent line to $\mathcal{U} = \text{const}$ is such that $0 = d\mathcal{U} = d\Phi + m\omega_c (\omega_c x - \omega_c x_0) dx$, so, if $x = x_0$, then $d\mathcal{U} = d\Phi$. Therefore the two lines have the same equation. The property can be interpreted as follows: if $(x_0, y_0)$ is a point of the cathode and in this point an electron with zero velocity is emitted $(p_x = p_y = 0, p_z = -m\omega_c x_0)$, then the electron moves in a part of the phase-space such that $\mathcal{H} = q\Phi(x_0, y_0) = \mathcal{U}(x_0, y_0)$. Being $\mathcal{H}(x, y, p_x, p_y) \geq \mathcal{U}(x, y)$, the region of $\mathbb{R}^2$ in which the electron can be found must satisfy the condition

$$\mathcal{U} (x, y) < \epsilon = \mathcal{U} (x_0, y_0)$$

and it is delimited by the curve $\mathcal{U}(x, y) = \mathcal{U}(x_0, y_0)$. In addition, if the curves $\Phi(x, y) = \Phi(x_0, y_0)$ and $\mathcal{U}(x, y) = \mathcal{U}(x_0, y_0)$ were not tangent in $(x_0, y_0)$, the region of the motion, eq. (7), should have points in the region $q\Phi(x, y) > q\Phi(x_0, y_0)$, but this is impossible being

$$\epsilon = q\Phi(x, y) + \frac{1}{2}mv^2 = q\Phi(x_0, y_0) \Rightarrow q\Phi(x, y) < q\Phi(x_0, y_0).$$

In the following, a particularly simple potential is considered, i.e.

$$q\Phi(x, y) = a^2 (y^2 - x^2).$$

This potential (which can be produced by using a pair of cathodes and a pair of anodes having a hyperbolic shape [5]) confines the electron only in the $y$ direction. The presence of a sufficiently strong magnetic field can confine the electron also in the $x$ direction, as the potential $\mathcal{U}$ assumes the form

$$\mathcal{U}(x, y) = \mathcal{U}_x(x) + \mathcal{U}_y(y) + \epsilon_m(p_z)$$

with

$$\mathcal{U}_x(x) = b^2 (x - x_m)^2, \quad \mathcal{U}_y(y) = a^2 y^2, \quad \epsilon_m(p_z) = -\frac{a^2 p_z^2}{2mb^2},$$

being $b^2 = m\omega_c^2/2 - a^2$ and $x_m(p_z) = -\omega_c p_z/(2b^2)$. The electron is confined in $x, y$ directions if $b^2 > 0$, i.e. if $|\omega_c| > a(2/m)^{1/2}$. From the Hamiltonian, eq. (10), uncoupled equations of harmonic oscillators for the motion in $x, y$ directions are obtained:

$$\frac{d^2 x}{dt^2} = -\omega_x^2 (x - x_m), \quad \omega_x = b \left(\frac{2}{m}\right)^{1/2},$$

$$\frac{d^2 y}{dt^2} = -\omega_y^2 y, \quad \omega_y = a \left(\frac{2}{m}\right)^{1/2}.$$
Therefore, the motion is confined in the rectangular region $\mathcal{R} \subset \mathbb{R}^2$ defined by

$$\mathcal{R} = \left[ x_m - \frac{\epsilon_x^{1/2}}{b}, x_m + \frac{\epsilon_x^{1/2}}{b} \right] \times \left[ -\frac{1/2 \epsilon_y}{a}, \frac{1/2 \epsilon_y}{a} \right],$$

where $\epsilon_x, \epsilon_y$ are the energies associated to the oscillatory motion in $x$ and $y$ directions, respectively (the total energy, $\epsilon$, is simply given by $\epsilon = \epsilon_x + \epsilon_y + \epsilon_m(p_z)$). If the ratio between $a$ and $b$ is not a rational number, the trajectory covers totally the region $\mathcal{R}$ (as shown in fig. 1). Figure 2 shows the elliptic region defined by eq. (7) and the corresponding region $\mathcal{R}$ for an electron emitted by the cathode. According to the theory, the ellipse is tangent to the cathode.

3. – Averaged densities and collision frequencies

In the physical situation here considered, the collision frequency is much smaller with respect to the characteristic frequencies of the motion. Therefore, instead of calculating the instantaneous position of the electron at each time instant, one can consider the time average of the trajectory [6]. In terms of particle density the results obtained with this technique are extremely accurate, as they differ from the real ones only because of microfluctuations of the density (occurring on the time scale of the oscillation period) and can be regarded as reference solutions for the problem. In the case of the separable potential (11), one can express the time-averaged phase-space distribution associated to the electron motion as

$$f_A(x, p) = C \cdot \delta \left( \frac{p_x^2}{2m} + \mathcal{W}_x(x) - \epsilon_x \right) \delta \left( \frac{p_y^2}{2m} + \mathcal{W}_y(y) - \epsilon_y \right).$$
Fig. 2. – Curves $\Phi(x, y) = \text{const}$ in the region between the electrodes for the hyperbolic potential, eq. (9). The rectangular and elliptic regions show the support of density distributions $\rho_A$ and $\rho_E$, respectively, for an electron emitted from the cathode at $x = x_0$.

\[
\begin{align*}
\text{cathode} & \quad \text{anode} \\
\text{anode} & \quad \text{cathode}
\end{align*}
\]

(\text{the constant} \ C \ \text{is such that} \ \iint f_A \, dx \, dp = 1). \ \text{From} \ f_A, \ \text{the space density,} \ \rho_A = \int f_A \, dp, \ \text{can be factorized as}

\[
(15) \quad \rho_A(x) = \rho_x(x) \rho_y(y)
\]

\[
(16) \quad \rho_x(x) = \begin{cases} 
\frac{b}{\pi} \left[ \epsilon_x - b^2 (x - x_m)^2 \right]^{-1/2}, & |x - x_m| < \frac{\epsilon_x^{1/2}}{b} \\
0, & \text{otherwise}
\end{cases}
\]

\[
(17) \quad \rho_y(y) = \begin{cases} 
\frac{a}{\pi} \left[ \epsilon_y - a^2 y^2 \right]^{-1/2}, & |y| < \frac{\epsilon_y^{1/2}}{a} \\
0, & \text{otherwise}
\end{cases}
\]

Local concentrations of charge inside the device may behave like scattering centers. When a Coulomb scattering event happens, the total energy $\epsilon$ is unchanged but with a different distribution between $\epsilon_x$ and $\epsilon_y$. The final effect of multiple scattering is creating an ergodic distribution in the phase space. In this case, the correct time-averaged phase space density is the following:

\[
(18) \quad f_E(x, p) = C \cdot \delta \left( \frac{p^2}{2m} + \mathcal{V}(x) - \epsilon \right)
\]

and the space distribution is given by

\[
(19) \quad \rho_E(x) = \begin{cases} 
\frac{1}{\mathcal{A}(\epsilon, p_z)}, & \mathcal{V}(x) \leq \epsilon \\
0, & \mathcal{V}(x) > \epsilon
\end{cases}
\]
\[ \mathcal{A}(\epsilon, p_z) = \int_{W(x, p_x) \leq \delta} \text{d}x \text{ being the area of the permitted region of motion. From the above introduced densities, the time-averaged collision frequencies can be calculated. The instantaneous collision frequency for a single electron is } \nu(t) = v(t)\sigma(v(t)). \mathcal{N}_a, \mathcal{N}_b \text{ being the atom density and } \sigma(v) \text{ the cross-section of the considered process. Instead, the averaged frequency, } \bar{\nu}, \text{ is given by}
\]

\[ \bar{\nu} = \int \int v \sigma(v) \mathcal{N}_a f(x, p) \text{d}x \text{d}p\]

being \( v(\epsilon, x) = \left[ 2m(\epsilon - q\Phi(x)) \right]^{1/2} \). In particular, using the ergodic distribution, \( f_E \), one obtains

\[ \bar{\nu}_E (\epsilon, p_z) = \int dx \int_0^{+\infty} v \sigma(v) \mathcal{N}_a C \delta \left( \frac{p^2}{2m} + U(x) - \epsilon \right) 2\pi p dp \]

\[ = \int v(\epsilon, x) \sigma(v(\epsilon, x)) \mathcal{N}_a \rho_E (x; \epsilon, p_z) \text{d}x. \]

A similar result is obtained using the other distribution, \( f_A \); in fact, the time-averaged frequency \( \bar{\nu}_A (\epsilon_x, \epsilon_y, p_z) \) is obtained from eq. (21) by replacing \( \rho_E \) with \( \rho_A \).

4. – Effect of the collisions

When phenomena having time scales much larger than the ones characterizing the electron motion are considered, each electron can be regarded not as a point particle but as having a spatial charge distribution, according to eq. (15) or eq. (19), having collision frequency provided by eq. (20). In this way, each electron is fully described by indicating the set of its constants of the motion, \( \{ \epsilon_x, \epsilon_y, p_z \} \) or \( \{ \epsilon, p_z \} \). When an elastic collision happens, the electron changes its parameters. If the collision has place in \( x_P \), the electron has velocity \( v(\epsilon, x_P) \) and therefore the (density) probability of the event is \( v(\epsilon, x_P)\sigma_{el}(v(\epsilon, x_P))\mathcal{N}_a/\bar{\nu}_a \). By considering that the masses of the atoms are much larger than the electron mass, after a collision the electron has velocity \( \mathbf{v} = v\Omega' \), where \( \Omega' \) is a random unit vector, and its trajectory is described by a set of new constants of the motion, \( \{ \epsilon', p_z' \} \), or \( \{ \epsilon_x, \epsilon_y, p_z' \} \). More specifically

\[ \epsilon' = \epsilon, \quad p_z' = m(v_z' - \omega_c x_P), \]

\[ \epsilon_y' = \frac{m}{2}v_y'^2 + a^2 y_P'^2, \quad \epsilon_x' = \epsilon - \epsilon_y' - \epsilon_m(p_z'). \]

An ionization event may happen in \( x_P \) (with density probability \( v(\epsilon, x_P)\sigma_{i}(v(\epsilon, x_P))/\bar{\nu}_i \)) only if \( \frac{1}{2}mv^2(\epsilon, x_P) \) is greater than the ionization energy, \( \epsilon_i \). In this case, one must calculate the constants of motion of the primary (a) and secondary (b) electrons, as

(a) \( v'_a = (v^2 - 2\epsilon_i/m)^{1/2}, \quad \mathbf{v}'_a = v'_a\Omega' \),

\[ \epsilon'_a = \epsilon - \epsilon_i, \quad p'_{a, x} = m(v'_{a, x} - \omega_c x_P), \]

\[ \epsilon'_{y, a} = \frac{m}{2}(v'_{y, a})^2 + a^2 y_P'^2, \quad \epsilon'_{a, x} = \epsilon'_a - \epsilon_{y, a} - \epsilon_m(p'_{z, a}); \]

(b) \( v'_b = 0 \),

\[ \epsilon'_b = q\Phi(x_P), \quad p'_{b, x} = -m\omega_c x_P, \]

\[ \epsilon'_{y, b} = a^2 y_P'^2, \quad \epsilon'_{x, b} = \epsilon'_b - \epsilon'_{y, a} - \epsilon_m(p'_{z, b}). \]
Fig. 3. – Comparison between the charge distribution obtained using the ergodic technique (based on the distribution $\rho_E$, upper part of the figure) and the time-averaged distribution (based on the distribution $\rho_A$, lower part of the figure), after 3.4 ms from electrons injection. Only elastic collisions are considered ($\nu_{el} = 3$ kHz).

5. – Numerical technique

The above presented theory suggests a possible numerical technique for studying the dynamics of the electrons density due to collisions with neutral atoms. Initially, a set of $N$ computational particles is generated having zero velocity at different positions of the cathode (in order to simulate the electron emission due to field effect) and the relative

Fig. 4. – Comparison of charge distributions after 0.68 ms when the anode is far from the region of interest and the electrons are not removed. In the figure, the distribution obtained with the ergodic technique is represented in the upper part, while the time-averaged distribution in the lower part. Only elastic collisions are considered ($\nu_{el} = 3$ kHz).
set of $2N$ (for the ergodic technique) or $3N$ (for the time-average method) parameters is calculated. Then, at each time step a subset of colliding particles is selected by using a Monte Carlo technique. For each colliding electron, the type of collision (elastic or ionization), the spatial position of the event and the new direction $\Omega'$ are chosen. In this way, the set of characteristic parameters of the set of computational particles is updated at each time step, as described in sect. 4. If the anode intersects the region occupied by the electron, then the particle is removed.

Typical results obtained with this method are presented in figs. 3 and 4. In fig. 3, the charge density is shown for electrons emitted by the cathodes in the interval $0 < x < 1$ mm after a transient of 3.4 ms. A minimum difference between the (approximated) ergodic method and the time-average method (which can be regarded as the reference result) can be evidenced only in the region close to the anode, as the ergodic distribution occupies a larger domain (as shown in fig. 2) and therefore the probability for an electron to be absorbed by the anodes is greater. This fact is confirmed in fig. 4, where a similar case is considered in which the anodes are far from the region of interest and consequently the main cause of discrepancy between the two methods disappears.

The study here presented is simplified as the effect of the self-consistent electric field is neglected. However, in principle this effect can be included into the calculation. In particular, if the ergodic technique is employed, at each time step the self-consistent potential must be recalculated, and the energies of the particle must be updated by imposing the conservation of the ergodic invariant [1].

REFERENCES